

Report of Independent Studies

Performed under the supervision of Tom DeGrand

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Simulation of Transition and Phase Separation in ^3He - ^4He Mixtures

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Abstract

This paper is the final report of the Independent Studies under supervision of Professor Tom DeGrand at the University of Colorado. The topic deals with a paper located back in 1971, which has been written by Blume, Emery and Griffiths¹. Even though their paper contained some unphysical properties the overall result was quite remarkable, taking also in consideration that they evaluated everything analytically in Mean-Field-Theory. The task in this Fall Term 2010 for the Independent Studies was to confirm or correct their research results by using a Monte-Carlo based simulation with the Heat-Bath algorithm.

In the end the main goal was to evaluate the results of the simulation so that the paper of Friedan, Qiu and Shenker³ could be confirmed or corrected. The authors of this paper state that at the Tricritical point, where the phase transition goes from second to first order, we have a supersymmetrical system, i.e. our critical exponents should have the values of a supersymmetrical system. To do this research we need to work with finite size scaling and gather a lot of data along the critical line of this system.

I. INTRODUCTION

^3He - ^4He -Mixtures are very important for cooling systems having to provide temperatures lower than 1 K. The process where these mixtures are used is called dilution refrigeration. The physical background is that by mixing these isotopes of Helium energy is being consumed by the system - energy in form of temperature. In more detail, energy is required to transport the ^3He atoms from the ^3He -rich phase into the ^3He -poor phase. If the atoms can be made to continuously cross this boundary, they effectively cool the mixture. Because the ^3He -poor phase cannot have less than a few ^3He percent at equilibrium, even at absolute zero, dilution refrigeration can be effective at very low temperatures. The volume in which this takes place is known as the mixing chamber. Even though this kind of system has been studied very well experimentally, the theoretical framework is still missing or incomplete. An approach in form of an Ising Model has been introduced by Blume, Emery and Griffiths (1971)¹. They propose a modified Ising Hamiltonian as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - K \sum_{\langle i,j \rangle} s_i^2 s_j^2 + \Delta \sum_i s_i^2 - N(zK_{33} + \mu_3). \quad (1)$$

The spin can take the values $0, \pm 1$ in this model, assigning $0 \rightarrow ^3\text{He}$ and $\pm 1 \rightarrow ^4\text{He}$. Thus as in the standard Ising model the average of the total spin is given by (where N denotes the total number of sites)

$$M = \frac{1}{N} \sum_{i=1}^N \langle s_i \rangle. \quad (2)$$

Since we have now two different types of *atoms* in the system we need to distinguish between them. We can obtain the number of ^3He , N_3 , and ^4He , N_4 , atoms by calculating

$$N_3 = \sum_{i=1}^N (1 - s_i^2), \quad (3)$$

$$N_4 = \sum_{i=1}^N s_i^2. \quad (4)$$

The Hamiltonian described in eq. 1 is not very useful to evaluate. Since the paper of Blume, Emery and Griffiths (1971)¹ only deals with $J \gg K$ we use $K \approx 0$. Our unit set will be $J = 1$, and $\Delta = \mu_3 - \mu_4 \equiv -\mu$ in units of J . The later comes from our approximation $\mu_3 = 0$. Therefore our Hamiltonian looks like

$$\mathcal{H} = - \sum_{\langle i,j \rangle} s_i s_j - \mu \sum_{i=1}^N s_i^2. \quad (5)$$

Most statistics we are interested in are analogous to the standard Ising model. Next to the ones already mentioned (the internal energy of the system can be calculated by using the Hamiltonian from eq. 5, the “magnetization” of the system can be evaluated using eq. 2 and the particle number observables are already written down explicitly) we can use the specific heat C which is given as the variance of the energy, i.e.

$$C = \beta^2 (\langle E^2 \rangle - \langle E \rangle^2) = \frac{\partial E}{\partial T}. \quad (6)$$

The usage of this observable will be very important for finding the critical line (β_c, μ_c) as well as detecting the Tricritical point in that line, β_{tc}, μ_{tc} . We can also use C to measure the critical exponent ν . Another very important statistic will be the magnetic susceptibility, which can be evaluated by using

$$\chi = \beta (\langle M^2 \rangle - \langle M \rangle^2) = \frac{\partial M}{\partial \beta}. \quad (7)$$

This statistic has a very deep meaning for this research, because by evaluating plots and data of χ we will be able to get out the critical exponent γ . In the end we will focus completely on γ in order to proof or counter-proof the existence of Supersymmetry at the Tricritical point of a Tricritical Ising model as the one we study in this case.

II. MEAN FIELD THEORY

The original paper by Blume, Emery and Griffiths (1971)¹ made some approximations in order to use Mean Field Theory for obtaining analytical results. Even though the exact derivations and assumptions are irrelevant for us, the results are quite important since we need to confirm or correct them. The phase diagram shown in the paper (fig. 1) is an analytic approach to the experimentally

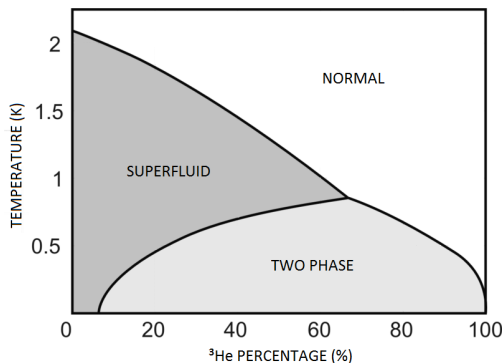


FIG. 1: Qualitative experimental phase diagram for the mixing process

measured phase diagram shown in fig. 1. By comparison we see directly that the scaling of the analytic approach does not fit the experimental data for $J \equiv 1$. Therefore we can already predict that the scaling of all analytic derived results in the paper by Blume (1971)¹ will not fit to our results, where we set $J \equiv 1$.

On the other hand we should be able to compare our results with the results of the paper qualitatively. Another interesting plot is shown on page 1075 (fig. 3), where the critical line (β_c, μ_c) is displayed. We are able to verify this behavior of $\mu_c(\beta_c)$ with the help of the given analytic equation,

$$\mu_c = -\frac{1}{\beta_c} \ln(\beta_c - 1), \quad (8)$$

which can only be evaluated for $\beta_c > 1$. The main problem for verifying this equation will be the different scaling for J used by the analytic approach compared to our simulation. We will try to adjust the scaling when doing the comparison in order to be able to match the analytic and numerical values as best as possible.

III. THE SIMULATION

The simulation uses a Monte-Carlo approach to the problem in form of an Heat-Bath algorithm as presented in Tom DeGrands book² on page 145 and 146. Since the simulation was only required to run on a specific computer the choice for the programming language was C#. The advantages of this choice are

- C like syntax combined with modern advantages like object-oriented programming,
- full access to the .NET-Framework in order to use graphical input controls,
- integrated file system access and
- direct access to the systems graphical output device in order to draw on the screen.

Even though some of these advantages are obsolete while programming physical simulations others are quite helpful in order to understand the physical system and optimizations. The program itself contained various possible functions such as

- running as simulation within a specific range of β values, as well as μ values,
- setting the number of iterations as well as warm-up-runs individually,
- setting the lattice size and number of repetitions,

- saving the output data in a textfile,
- having a first look at the statistics due to inbuilt data plotters and
- modify the raw output data in order to get specific statistic textfiles, which are more useful for evaluating the statistics than the raw data textfile.

Another feature of this program is the special simulation function, which runs the simulation for a specified amount of runs through a specific set of (β, μ) values, producing an own textfile in every run and for every (β, μ) value. This function was required in order to provide the necessary data background for running statistics beginning at the old Ising model (second order phase transition) and ending at the first order phase transition. This simulation produced 1,020 files (109 MB) running for nearly 24 hours straight (but only using one processor core, since the computer was needed for other tasks as well). The precision of this data was set to a very high level. The exact settings were:

- Every run for every value was done for every of these lattice sizes,

$$L \in \{16, 32, 48, 64\}, \quad (9)$$

representing L^2 number of sites.

- 5 runs each.
- Every run had 50 repetitions.
- Every repetition used 5000 iterations for each value.
- The number of warm-up-runs n was determined by the formula

$$n = 50000 \cdot \frac{L}{16}, \quad (10)$$

where L is the lattice size. This equation should of course be something like $L^2/16^2$ to be more accurate, but since several test runs at higher lattice sizes seemed to work fine with $n = 50000$ the only purpose of using this was to ensure that there are enough warm-up-runs for each lattice size.

Including all test and measure runs (to determine the critical line and approximately the Tricritical point) the overall number of files and filesize was already quite high, concerning a project of this size.

A. Algorithm

The main advantage of the Heat-Bath algorithm compared to the Metropolis et Al. algorithm used for deriving the former result of the standard 2D-Ising model lies in the processing speed. We can built a so called look-up-table for all possible cases of the model before iterating. Therefore the only task our simulation has to do is picking a random number and comparing this random number with the values from the look-up-table. That means that we gain all the time that was used to calculate the exponential function(s) in every iteration in the Metropolis et Al. algorithm. Following the book of Tom DeGrand² the Heat-Bath algorithm, which got his name from an analogy with a classical statistical ensemble, where the Hamiltonian and temperature are defined as $S(\phi) = H/k_B T$, visits each lattice site and replaces the value of the target site by a new value according to the probability distribution which will be generated beforehand and saved in a look-up-table.

The important part is that all values of the other sites are kept fixed. That we can use the look-up-table requires that the Heat-Bath transition probability is independent of the starting configuration ϕ , i.e.

$$R(\phi' \leftarrow \phi) \propto \exp(-S(\phi')). \quad (11)$$

This also implies that the ratio of the transition to the inverse transition satisfy this condition namely

$$\frac{R(\phi' \leftarrow \phi)}{R(\phi \leftarrow \phi')} = \frac{\exp(-S(\phi'))}{\exp(-S(\phi))}. \quad (12)$$

The pseudo-code for a Monte-Carlo step using the Heat-Bath algorithm is shown in the next code listing. To compute the total neighbor spins we use the same function as for the standard 2D-Ising model.

```
1 /* select random site at i,k and compute random number rand */
2 /* compute total neighbor spins S of site at i,k */
3 for(j=-1;j<2;j++)
4     if(rand<probability[j+1][S+4])
5     {
6         spin[i,k]=j;
7         break;
8     }
```

The most important part is the calculation of the probabilities, i.e. the computation of the look-up-table. For every (β, μ) value we need to re-compute the look-up-table, since the probabilities change due to a change in the Hamiltonian (we have $H \equiv H(\beta, \mu)$). The table can be presented as a 3×9 matrix, where the rows represent the different site values $(0, \pm 1)$, while the columns are matching the current state of the site. Therefore the usage of the matrix should be done as in the pseudo-code above, iterating through all the rows while keeping a specific column fixed, which has been determined through the calculation of the total neighbor spins.

```

1  /* create 3x9 array lookup */
2  for (int i = -4; i < 5; i++)
3  {
4    double norm = 0.0;
5    for (int j = -1; j < 2; j++)
6    {
7      lookup[j + 1, i + 4] = exp(beta * i * j + mu * beta * j * j);
8      norm += lookup[j + 1, i + 4];
9    }
10   for (int j = -1; j < 2; j++)
11     lookup[j + 1, i + 4] /= norm;
12 }

```

All probability entries are normalized to the sum of all entries in their row. The look-up-table must be global accessible that we are able to retrieve the necessary information doing a Monte-Carlo step.

B. Evaluation of first output

Before doing a more detailed and comprehensive evaluation it is very important to get a feeling for the system and (in this case) study the critical line in order to spot the Tricritical point. In order to find the critical line runs for different μ at different β values have been performed. Using a 3D plot the finding process is quite easy as shown in fig. 2.

Even though such plots can only be used in a qualitative way due to the lack of errorbars and lose of detail, it gives us a first impression about where maxima occur and where not. This information is quite helpful considering the fact that the simulation takes quite a long time to compute and we do not want to waste precious computing time in areas with nothing interesting going on. Instead we want to focus on the interesting parts in this system, i.e. the area around the change from

a second to a first order transition. With the help of these plots we can already tell where the

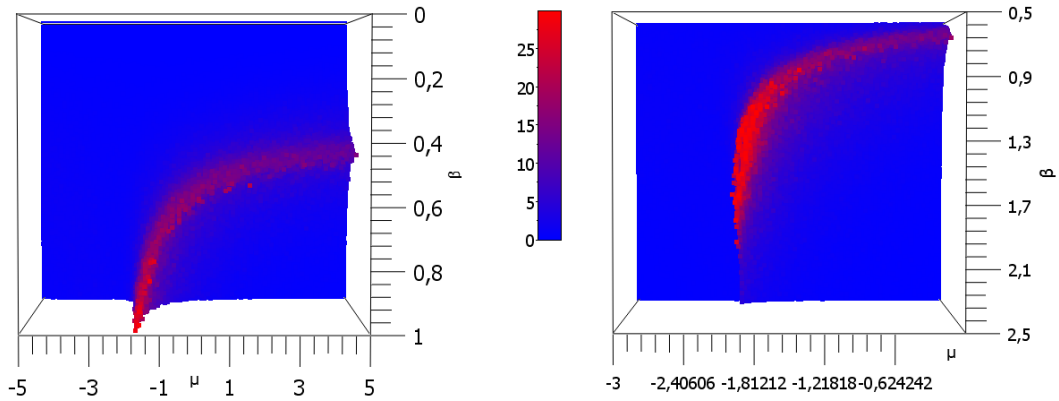


FIG. 2: 3D plot of the specific heat C in the $\beta - \mu$ plane to determine the critical line

critical line lies and where we have for sure a second order transition as well as where a first order transition occurs. To specify first or second order transition we can also use the value of H in a 3D plot. As we can see on the left image of fig. 3 at around a certain value of β we are getting a jump in the Hamiltonian. The right image gives us information about the value of μ . We see that the jump converges to a certain value of μ - meaning we have a straight line there. Once we know

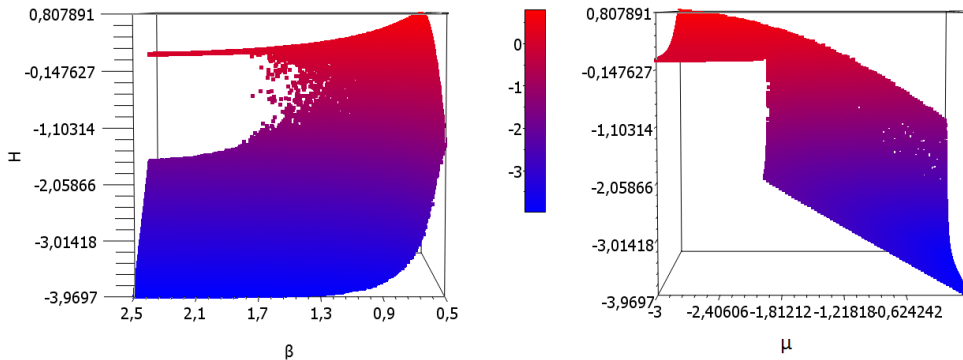


FIG. 3: 3D plot of the Hamiltonian H in the $\beta - \mu$ plane to determine the second / first order part

roughly about the location of the Tricritical point we can try to determine to as exact as required for our purposes. In order to do that we can and must use several techniques, which include the following:

1. Take slices of the 3D plot of the Hamiltonian H at fixed β and variable μ . Vary β and look when the plot starts to jump. We can determine the first order region due to the discontinuity.

2. By making a time history (in Monte-Carlo time, i.e. the number of iterations) at fixed μ, β we can determine if the tested point is actually in the first (jumps visible) or second (smooth value changes) phase transition.
3. Repeat the process at different lattice sizes L^2 . While H and C should be roughly the same in the first order region, finite size scaling effects will effect at least C in the second order phase transition region.
4. Another possible way is to do so called mixed-starts near the Tricritical region.

In our case we will use the first two techniques described above. Taking slices of H at $\beta = 0.9, 1.1, 1.3$ and $\beta = 1.4$ we see in fig. 4 that the Tricritical point must lie somewhere between $\beta = 1.1$ and $\beta = 1.4$. The reason for this assumption lies in the shape of the plots. While the first

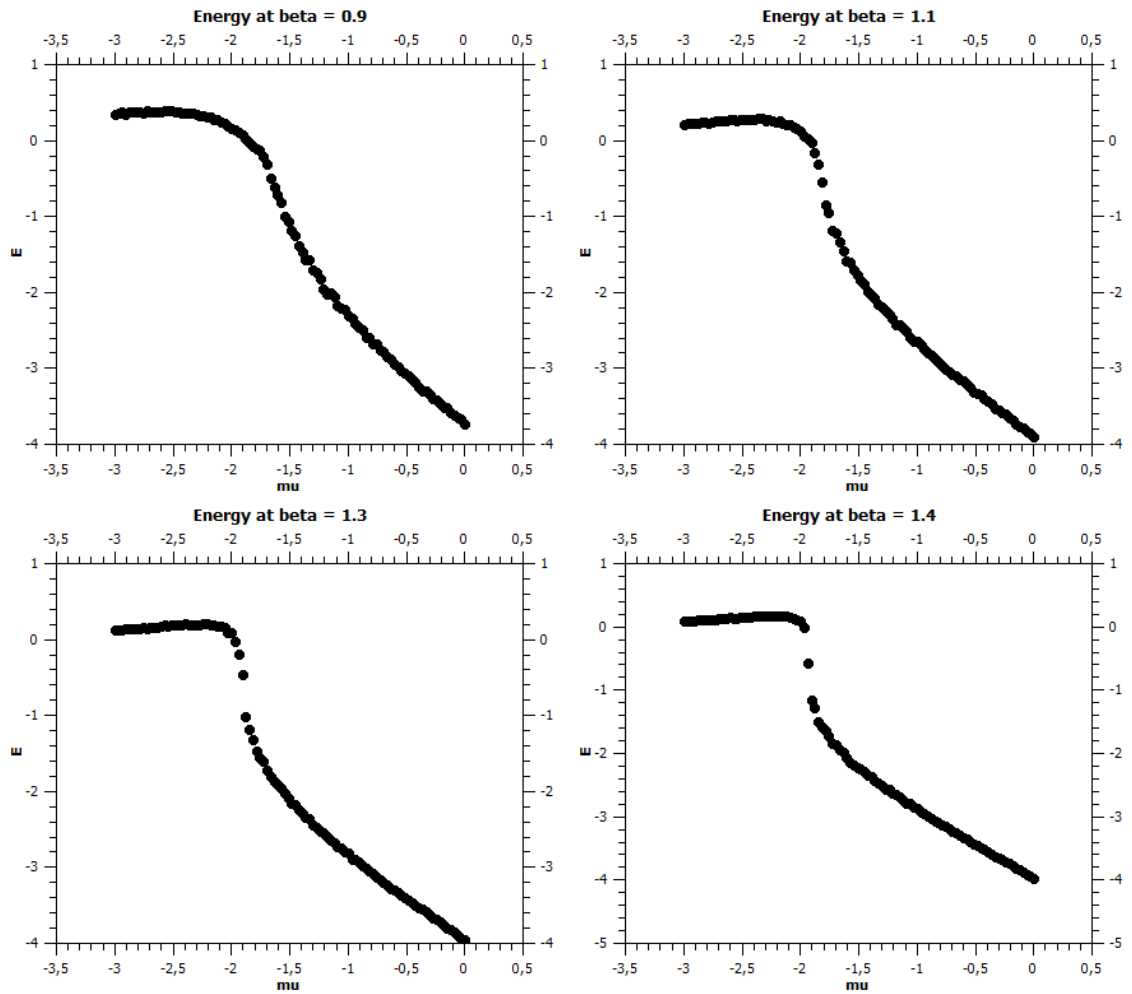


FIG. 4: Slices of the Hamiltonian beginning at top left $\beta = 0.9, 1.1, 1.3$ and ending at bottom right $\beta = 1.4$

one shown in fig. 4 has a smooth slope, the slope in the other three ones is getting steeper and

steeper. The question after this analyzation is where exactly is the slope so steep that it can be considered a discontinuity and marks the Tricritical point we are hunting after at the moment. To solve this puzzle we have to deal with another technique using Monte-Carlo time history. The advantage of this technique lies in the output given in form of $H(t)/N$, where t is the Monte-Carlo time. Even though the evaluation is kind of messy, since there are no totally clear indicators for either side, a lot of evaluation time has to be done interpreting the plots and looking for details. Fig. 5 shows a comparison of different Monte-Carlo time history snapshots taken with a warm-

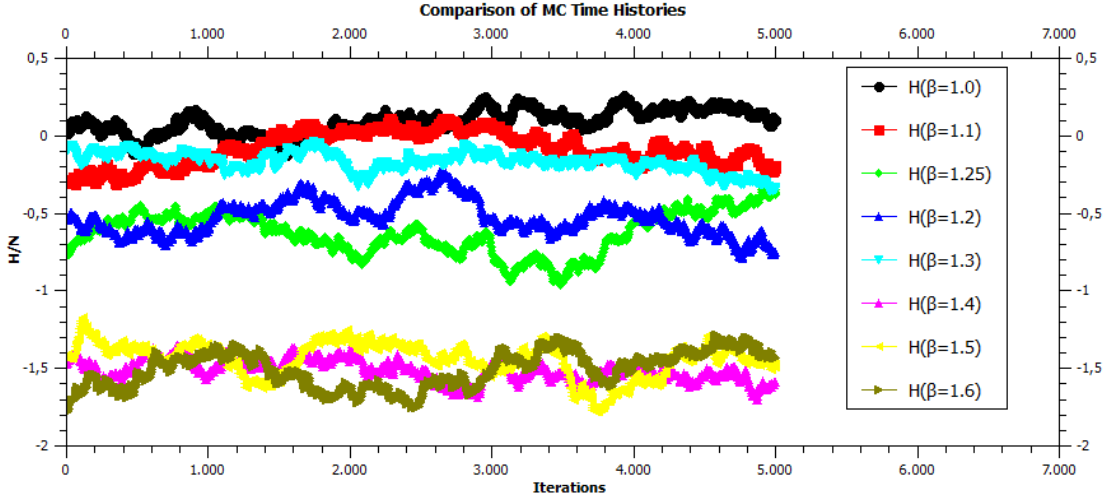


FIG. 5: Comparison of different time histories of H/N at β, μ pairs lying approx. on the critical line

up-length of 50000 iterations and a runtime of 5000 iterations. We directly see a few important details:

- We can group the different plots to two or three groups. The lower three graphs ($\beta = 1.4, 1.5, 1.6$), the two graphs in the middle ($\beta = 1.2, 1.25$) and the upper three graphs ($\beta = 1.0, 1.1, 1.3$) form these groups.
- The shape of the graphs look very different overall. While graphs below $\beta = 1.2$ show smooth transitions, the upper ones, especially $\beta = 1.25$, provide the strong variations as expected beforehand.
- The H/N gap between $\beta = 1.3$ and $\beta = 1.4$ is remarkable.
- The plot of $\beta = 1.3$ is the only one going up in H/N compared to its predecessor- β -wise, i.e. $\beta = 1.3$ has an higher value of H/N in average than $\beta = 1.25$ had.

- The lowest group consistent of $\beta = 1.4, 1.5, 1.6$ shows nearly the same behavior and has nearly the same average value in H/N .

The interpretation of these details is not that easy as it seems at first since some properties seem to contradict some of the properties already thought to be understood. To be sure not to make any mistakes we can use another set of evaluations concerning the specific heat C . In fig. 6 we can

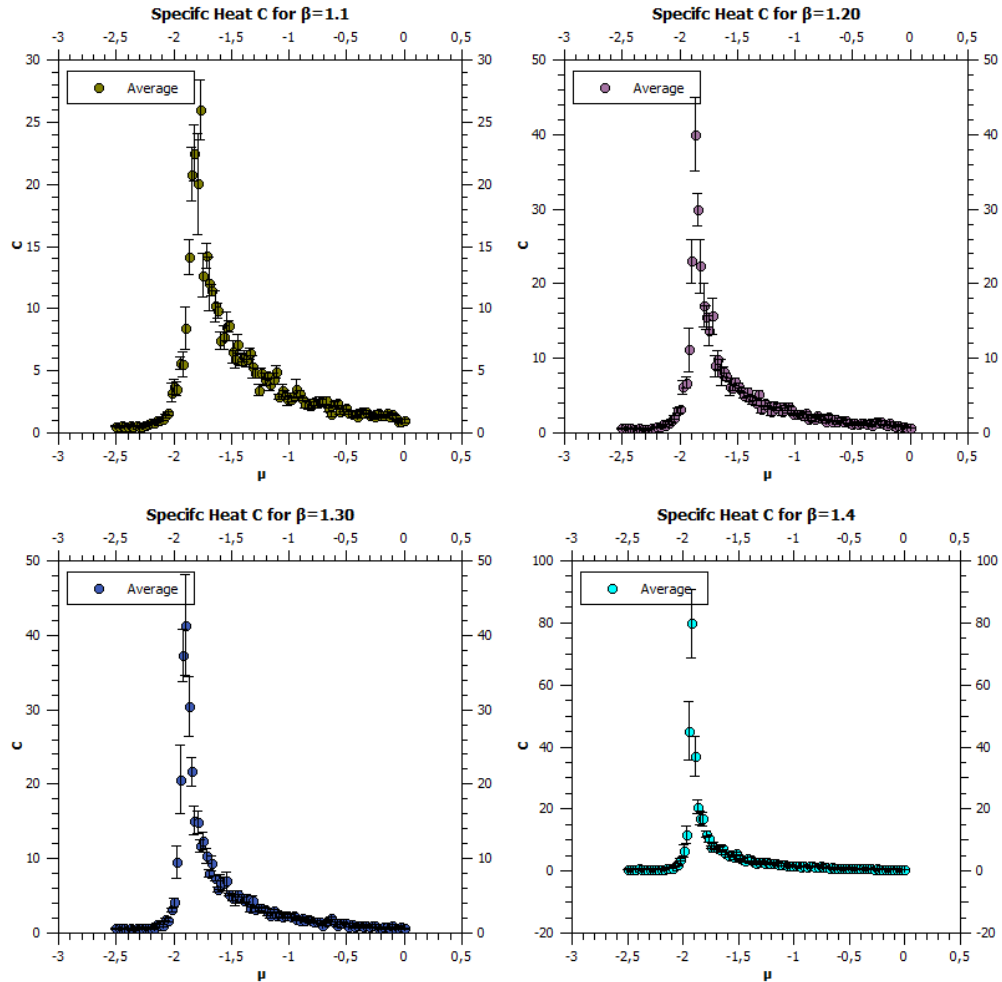


FIG. 6: Slices of the specific heat C beginning at top left $\beta = 1.1, 1.2, 1.3$ and ending at bottom right $\beta = 1.4$

see that between the values of $\beta = 1.3$ and $\beta = 1.4$ something strange happens. The peak in the specific heat shows a very clear discontinuity at $\beta \geq 1.4$, while the peak at $\beta \leq 1.3$ behaves as we expect from the standard Ising model. This gives us reason (along with the time history and the Hamiltonian) to justify that the first order transition must be around the value of $\beta = 1.3$.

Now that we determined the critical line and now that we have a rough imagination where the Tricritical point is located, we can start a more detailed evaluation.

C. A more detailed evaluation

Our first task in a more detailed evaluation is to fix the Tricritical point as close as possible. We will use the last technique presented in the previous section, evaluating the specific heat C for a set of certain values of β . At the Tricritical point we will see a strong change in the shape of C , along with a discontinuity showing up. Our evaluation was based in the range of $\beta \in [1.3, 1.35]$. While the plots of the specific heat from $\beta = 1.3$ until $\beta = 1.33$ do not show any of the shape

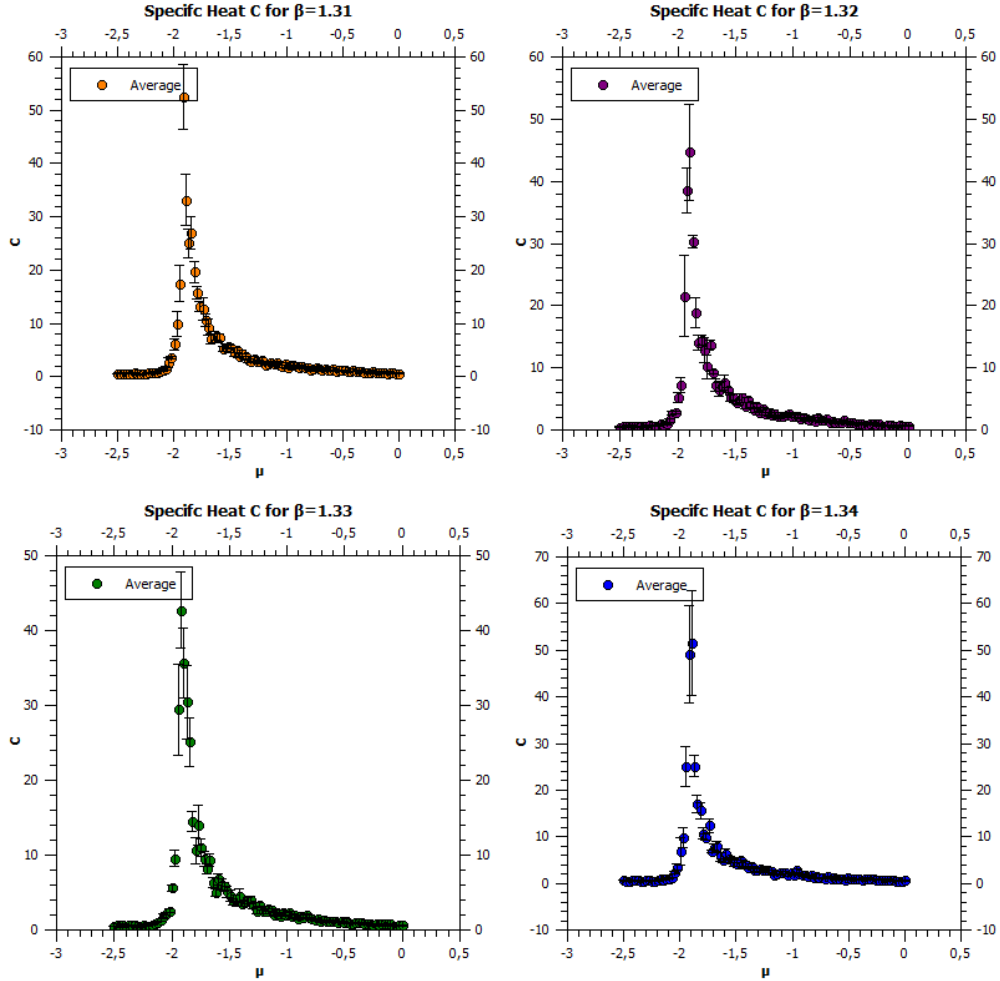


FIG. 7: Slices of the specific heat C beginning at top left $\beta = 1.31, 1.32, 1.33$ and ending at bottom right $\beta = 1.34$

changes mentioned above, the plot for $\beta = 1.34$ certainly does - see fig. 7. We therefore conclude that the Tricritical point is certainly reached at $\beta = 1.34$ and will stay below that β value. If we take that last plot as reference we are able to determine the Tricritical point using the peak value

of the specific heat. We did find that

$$(\beta_c, \mu_c) \equiv (1.34, -1, 89). \quad (13)$$

For all further evaluations we will stay above μ_c and below β_c . We now have to determine the characteristics of the plots evaluated in the fig. 6 and 7. We remark that:

- The errorbars increase for $\beta \geq 1.32$.
- The maximum for $\beta \leq 1.32$ is always in the same range (including errorbars).
- The discontinuity is visible for $\beta \geq 1.34$ interpolating a curve.
- The FWHM is approx. constant before $\beta = 1.34$ and goes to zero at the Tricritical point.
- The maximum value lies always under 60 for $\beta \leq 1.33$ - oscillating around with errorbars being in range.
- The maximum suddenly goes over 60 for $\beta \geq 1.34$ (including errorbars) and keeps rising (see $\beta = 1.4$).

We are now also interested in the changes of other observables. Since our aim is to get the critical exponents in order to compare these to the papers of Privman (1984)⁵, Friedan (1984)³ and Friedan (1985)⁴, as well as Lee (2007)⁷, we are interested in plots of the susceptibility χ . We expect a similar behavior of those as we had with the specific heat C . The plots in fig. 8 show on the side a different

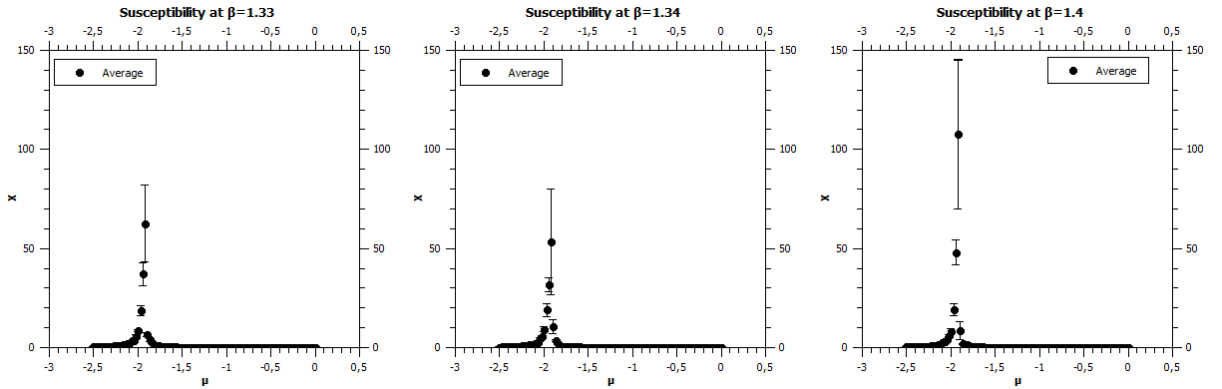


FIG. 8: Plots of the susceptibility χ from left $\beta = 1.33, 1.34, 1.4$

picture than we expected, on the other side we are confirmed with our expectation. The plot for $\beta = 1.34$ shows now difference from the plot at $\beta = 1.33$ and also no difference for the plots in

$\beta \in [1.2, 1.32]$ (not shown here), while the plot for $\beta = 1.4$ (which as we have derivated is already in the first order transition) shows the characteristics that we have expected beforehand. We notice that the big difference in the first two plots is the value of the errorbar for the peak point. Since a main property of the Tricritical point is the oscillation and discontinuity (i.e. big errorbars), we are able to assume that even without clear evidences from these plots, the derivations from the other plots are still fine and therefore - even not that much obvious - we see our Tricritical point at the $\beta = 1.34$ plot again.

Before we step over to the evaluation of the Critical Exponents we want to verify some results of Blume (1971)¹. The first quantity was fig. 1, which can be verified by using the statistics of N_3 as described in eq. 3. In fig. 9 we see a special view on a 3D plot showing $\beta, \mu, N_3(\beta, \mu)$. Only using

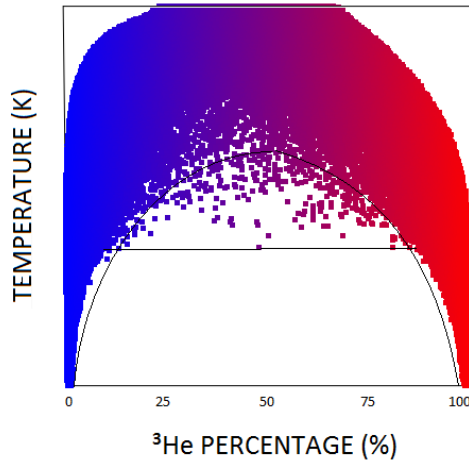


FIG. 9: A 3D plot for showing N_3 projected to the β plane only

the projection of this plot, i.e. β as y axis and N_3 as x axis we obtain the picture shown. This means we only used μ to compute the values and compressed the whole μ plane to one dot, i.e. reducing the plot dimensions from 3 to 2 since μ is just a computation helper (variation in μ gives us the different values), and not a real variable varied in experiments. In order to see some things better we have inserted very small black lines. These lines represent the boundaries of the phases. The curved lines separate stable from not stable phases, the straight line separates the metastable from the instable phase. Therefore we can see that

- The white area below the straight line is stable.
- The partial dotted area above the straight line and below the curved lines is metastable.
- The rest is stable.

- The separation between superfluid and normal can only be done by further investigation / considering the μ plane.

The similarity between this plot and the experiment is remarkable. We can see that this model is actually able to describe the phase mixing of these mixtures very precisely. Another thing to verify from the Mean-Field-Theory Blume (1971)¹ did is the equation for the critical line, eq. 8. Even though the two curves in fig. 10 do not match, the similarity (especially in the upper part,

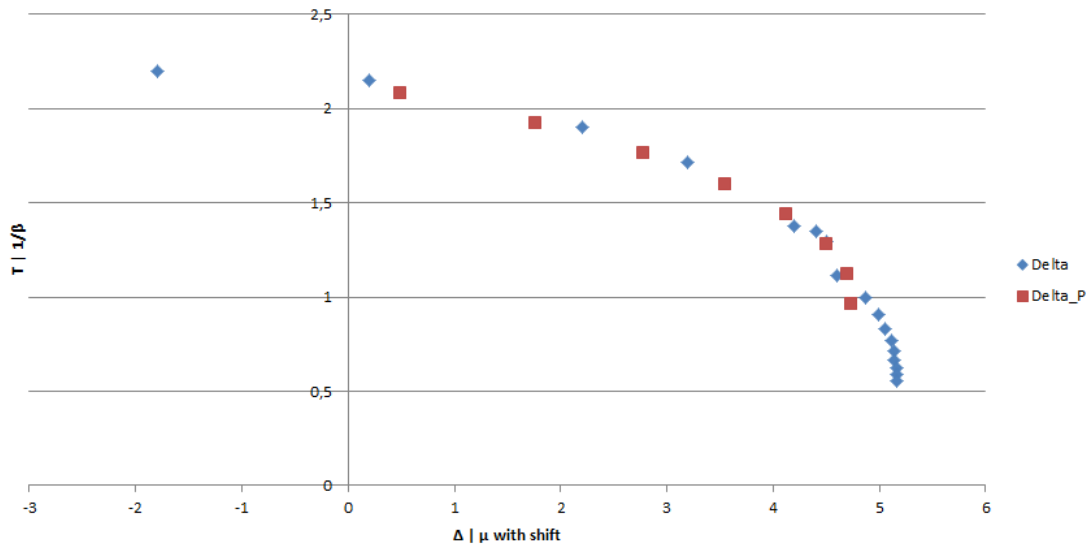


FIG. 10: Comparison of eq. 8 (DeltaP) to our measured values (Delta) (shifted by a const.)

above $T = 1.2$) is remarkable for an analytic equation in this case. Therefore we conclude that the equation of Blume (1971)¹ is a good approach which begins to fail commencing the first order transition.

A last thing we do want to have a look at is (since this is a more detailed evaluation) how the energy gap arises at the Tricritical point, i.e. what is happening between $\beta = 1.3$ and $\beta = 1.4$ in the plots of fig. 4. We already know that a discontinuity shows up - but (and that was our problem in the first case, i.e. getting the Tricritical point by only looking at the energy plots) we did not know when the discontinuity is the way it should be for the Tricritical point. Now that we determined the Tricritical point with the usage of other techniques we can use this information to gather some information about the changes of the energy at the Tricritical point by just comparing the plot at $\beta = 1.34$ with some plots before and after. The first thing we will notice are the very small errorbars in these plots - it is hard to see them at all. That means that the energy is - even at the Tricritical point - a very precise tool for measuring the state of the ensemble. In fig. 11 we see

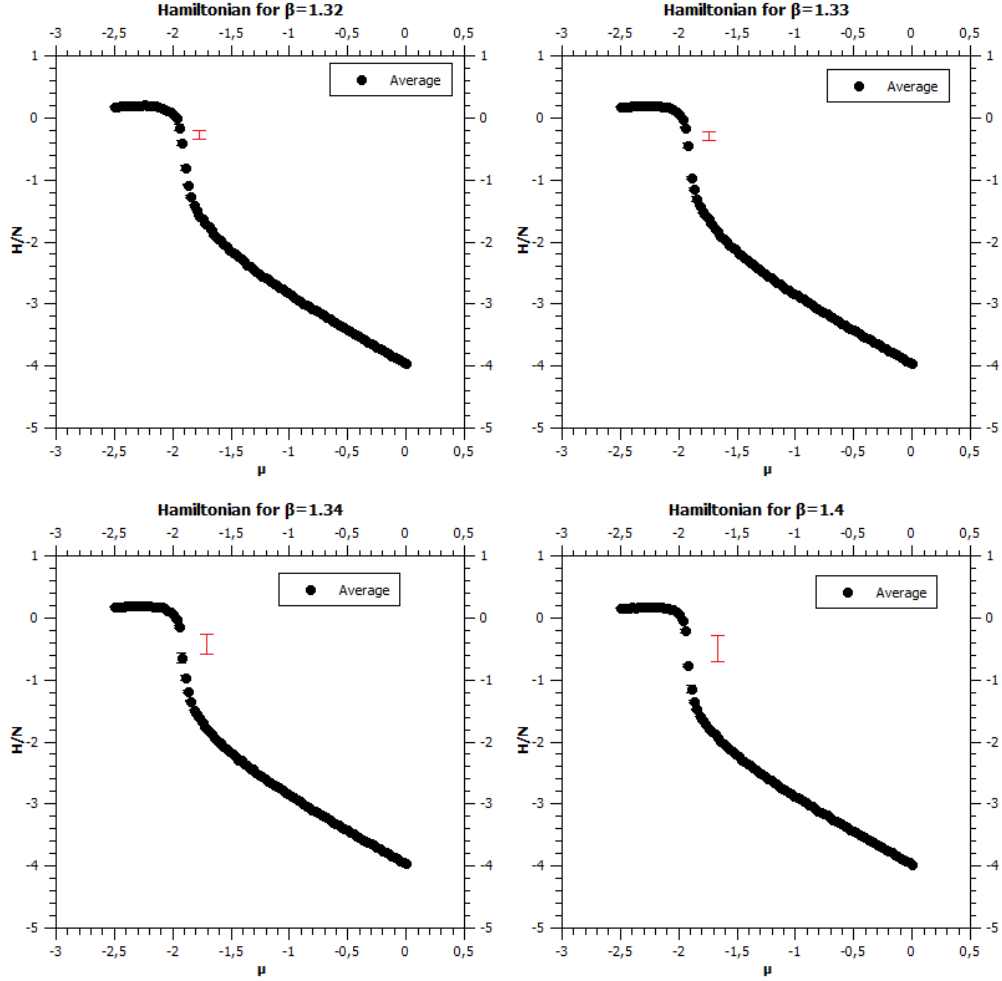


FIG. 11: Slices of the energy H beginning at top left $\beta = 1.32$, 1.33, 1.34 and ending at bottom right $\beta = 1.4$

that at the Tricritical point a gap arises (or the existing gap is getting bigger) between the upper edge and the first measured point after it. The important details are marked with red lines. We can therefore conclude that the gap shown before is in reality no gap, i.e. with an infinite amount of measured points we would get no gap, whereas the area between the horizontal red lines is a real discontinuity, which has opened up a little before and is (at the Tricritical point) then expanding.

D. Finite Size Scaling: Critical Exponents

Our main goal was to see how the critical exponents develop approaching a first order transition. For the finite size scaling methods we will follow the book of Cardy (1996)¹⁰ again as with the standard 2D Ising model. In the end we want to compare our critical exponents with the ones from

Friedan (1984)³, where the critical exponents are defined as

$$\langle O(z_1)O(z_2) \rangle \sim 1/|z_1 - z_2|^{2\Delta}. \quad (14)$$

The variable Δ is something like $x = h + \bar{h}$ in this case. In this equation the exponents are defined by the falloff of two-point-functions. Therefore we can get the Thermodynamic relations by integrating these functions a la Kubo, which will not be done here. The most relevant Z_2 (odd operator) has $\Delta = 2 \cdot (3/80)$, the most relevant Z_2 (even operator) has $\Delta = 2 \cdot (1/10)$.

A lot of the Supersymmetry relevant questions are in the more subtle properties, like the fact that the subleading relevant Z_2 (even operator) has $\Delta = 2 \cdot (1/10 + 1/2)$, where the $1/2$ is actually the spin of fermions. Getting back to our evaluation we will see while going to higher lattice sizes that the Tricritical point shifts a little bit in exactly the direction where wanted to take measures in. In

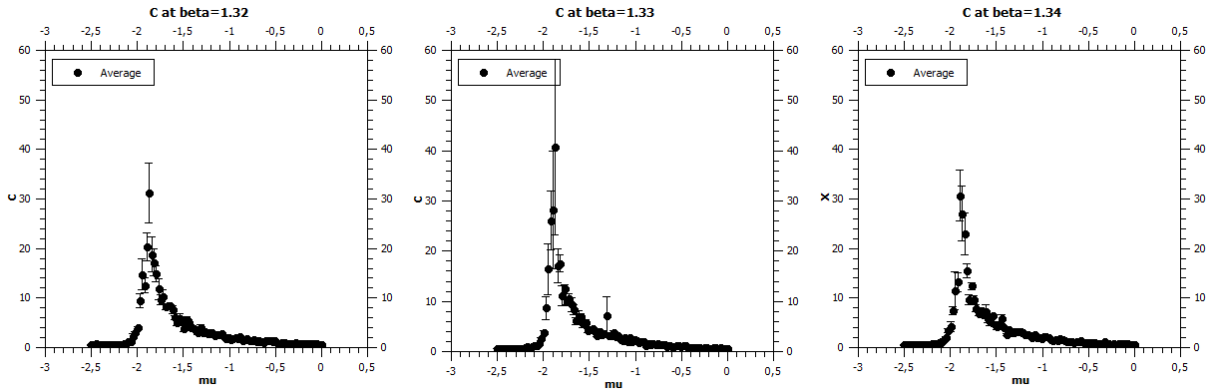


FIG. 12: Slices of the specific heat C in a 48×48 lattice at values $\beta = 1.32, 1.33, 1.34$

fig. 12 we see that the Tricritical point in a 48×48 lattice has been shifted to $\beta = 1.33$. Since we are interested in the development of the critical exponents while approaching the Tricritical point we will have to shift the evaluation back into another region, below $\beta = 1.32$ to be sure.

We will perform the evaluation of the critical exponents as before with the standard 2D Ising model. The main difference is that we will now perform not only one evaluation but several evaluations (for different values of β). We will include the following values of β ,

$$\beta \in \{1.28, 1.29, 1.30, 1.31\}. \quad (15)$$

The evaluation process of these values for lattice sizes L^2 with L being in the set

$$L \in \{16, 32, 48, 64\} \quad (16)$$

has been executed the following way:

1. Evaluation of χ and C at the values of β and L .
2. Determination of χ_{max} at μ_c for each plot, including $\Delta\chi_{max}$ for the error.
3. Determination of $FWHM(C)$ around C_{max} for each plot, including the error $\Delta FWHM(C)$.
4. Plot of χ_{max} vs. $FWHM(C)$ for each β with the values of all L .
5. Making a linear fit and determining the offset of the linear fit.
6. Collecting all offsets (including errors) and plotting γ vs β .

A set of plots for the specific heat in a 64×64 lattice is shown in fig. 13. By reading out the value

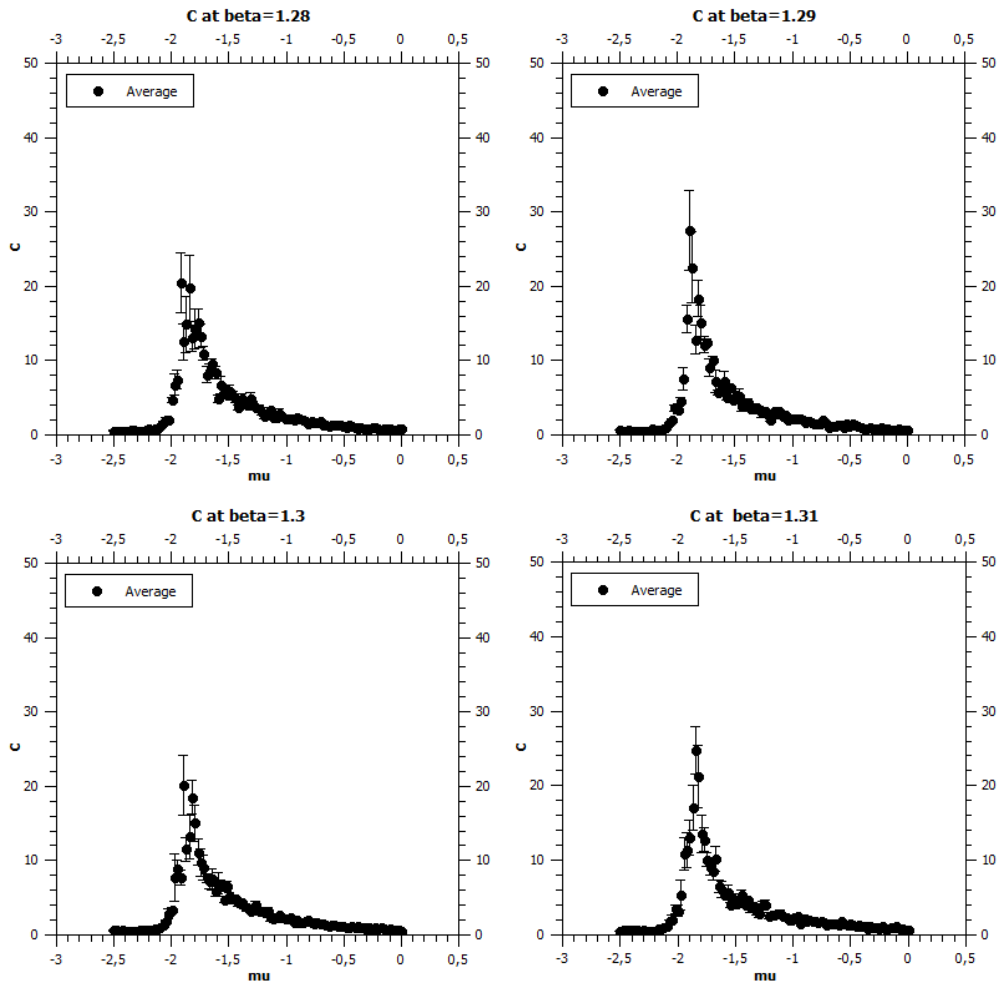


FIG. 13: Slices of the specific heat C in a 64×64 lattice at values $\beta = 1.28, 1.29, 1.30, 1.31$

of the maximum height we can determine at which height we have to search for the points left and right of the maximum to get the full width at half maximum. The error in this case was mostly

fixed to the precision of our measurements, i.e. the error was $2\Delta_\mu$, with Δ_μ being the difference between two measured values of μ (iteration step).

The other set of plots we are interested is shown in fig. 14. For the χ -plots we are reading out the

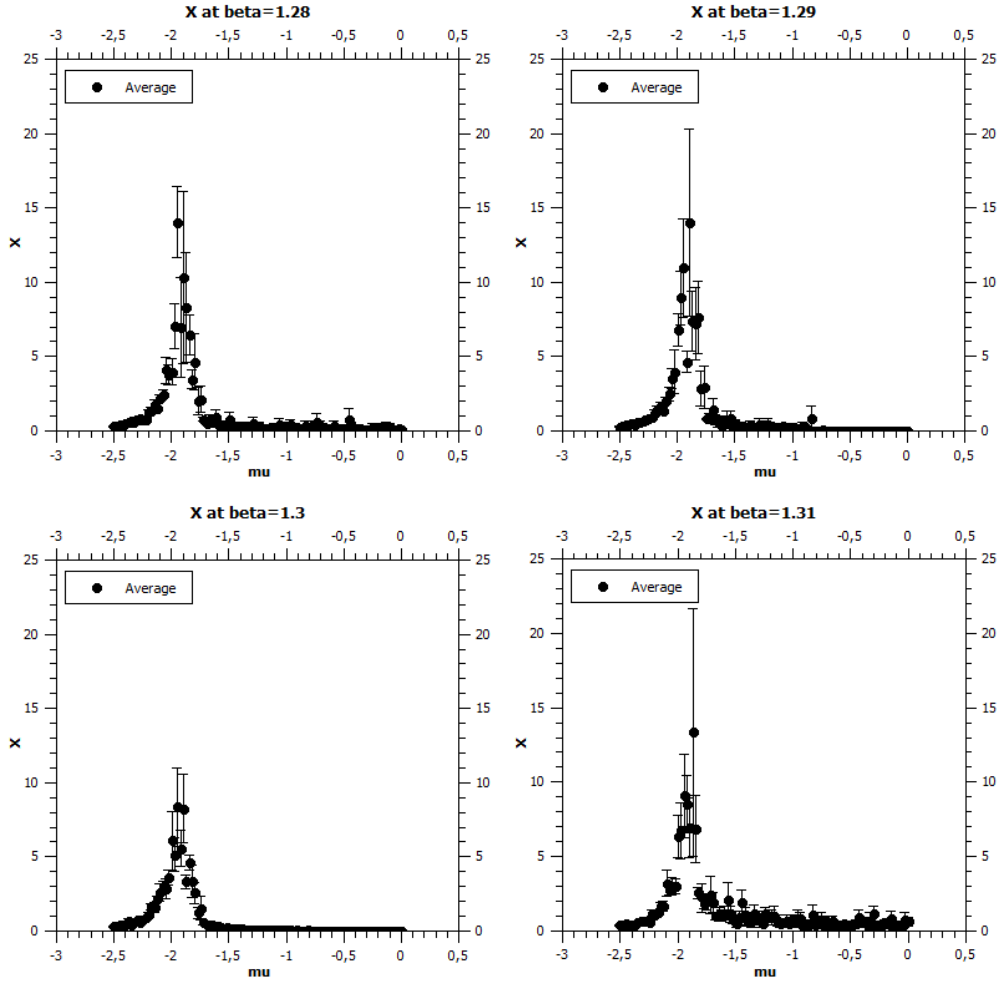


FIG. 14: Slices of the susceptibility χ in a 64×64 lattice at values $\beta = 1.28, 1.29, 1.30, 1.31$

height of the peak as well and additionally determine the error of the height due to the errorbar. The plot for the susceptibility shows some high oscillations approaching the Tricritical point, which makes the evaluation messy.

By fitting the final plot (γ vs β) with a linear approximation we obtain that the line is following the equation

$$\gamma(\beta) \approx -73 \cdot \beta + 95, \quad (17)$$

which is only an approximation because we had a very high error in these values. Overall we got for the slope a value of $A = (-73 \pm 240)$ and for the offset a value of $B = (95 \pm 310)$. A part of these

high errors could have been reduced by taking more evaluations into consideration or running the simulations even more below the Tricritical point. An interesting value can be obtained by setting γ to zero, i.e. finding the root of the function. We obtain

$$\beta_{tc} = 95/73 = 1.30. \quad (18)$$

This could be a hint that the Tricritical point is actually even before the point we evaluated (but then for all lattice sizes), and is just not so obvious to see in some low lattice sizes. Remarkable is that if we assume that $\gamma \approx 0$ is the Tricritical point, we obtain either a negative γ for a first order transition or a function of an higher order in general, since we would need at least a function $f(\beta^2)$ to get a minima and thus turning the sign of the derivative. But as we can see in fig. 15 the

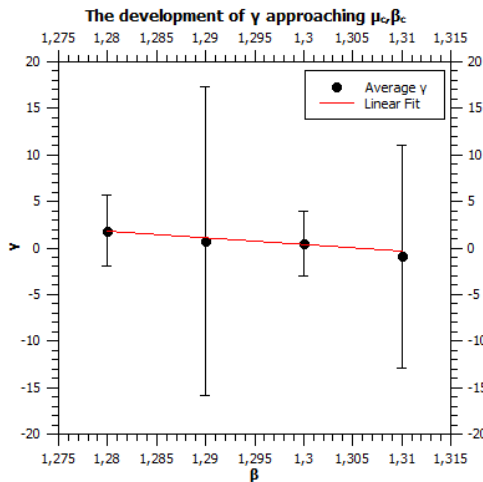


FIG. 15: The development of γ for different values of β

average values of γ give us the conclusion that (at least in the second order part of the transition) we really have a linear function representing $\gamma(\beta)$.

IV. CONCLUSION

The Hamiltonian \mathcal{H} from eq. 1, which was proposed by Blume, Emery and Griffiths (1971)¹ is really able to describe the mixtures of ${}^3He + {}^4He$ as we have seen using our Ising model based simulation. We could confirm most of their results and gather a lot of useful data. With this data it was possible to get even more realistic and useful results, e.g. the critical line.

The direct interpretation and evaluation of the critical exponents should be done in a further project since there is a lack of preparation and knowledge on my side. The data shows some

annoying features but also (if we ignore these properties) some very interesting results as presented with a linear fit. In the end we could have done a better evaluation by just using more values of β and L and shifting the direction to e.g. $\beta = 1.15$ until $\beta = 1.25$.

Acknowledgments

I want to thank Tom DeGrand for selecting this interesting topic, giving me fruitful advices on writing the actual simulation as well as providing me with literature and papers for further reading.

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- ¹ M. Blume, V. J. Emery and R. B. Griffiths, “Ising Model for the λ Transition and Phase Separation in He³-He⁴ Mixtures,” *Phys. Rev. A* **4(3)**, 1071 (1971).
 - ² T. DeGrand and C. DeTar, “Lattice Methods for Quantum Chromodynamics,” World Scientific Publishing, Singapore, ISBN **981-256-727-5**, (2006).
 - ³ D. Friedan, Z. Qiu and S. Shenker, “Conformal Invariance, Unitarity, and Critical Exponents in Two Dimensions,” *Phys. Rev. Lett.* **52(18)**, 1575 (1984).
 - ⁴ D. Friedan, Z. Qiu and S. Shenker, “Superconformal Invariance in Two Dimensions and the Tricritical Ising Model,” *Phys. Lett.* **151(1)**, 37 (1985).
 - ⁵ V. Privman and M. E. Fisher, “Universal critical amplitudes in finite-size scaling,” *Phys. Rev. B* **30(1)**, 322 (1984).
 - ⁶ M. N. Barber, R. B. Pearson, D. Toussaint and J. L. Richardson, “Finite-size scaling in the three-dimensional Ising model,” *Phys. Rev. B* **32(3)**, 1720 (1985).
 - ⁷ Sung-Sik Lee, “Emergence of supersymmetry at a critical point of a lattice model,” *Phys. Rev. B* **76(75)**, 103 (2007).
 - ⁸ R. Badke, “A Monte Carlo renormalisation group study of the two-dimensional discrete cubic model: a hint for superconformal invariance,” *J. Phys. A* **20**, 3425 (1987).
 - ⁹ M. E. Fisher and M. N. Barber, “Scaling Theory for Finite-Size Effects in the Critical Region,” *Phys. Rev. B* **28(23)**, 1516 (1972).
 - ¹⁰ J. Cardy, “Scaling and Renormalization in Statistical Physics,” Cambridge University Press, Cambridge, ISBN **052-149-959-3**, (1996).
 - ¹¹ L. Witthauer and M. Dieterle, “The Phase Transition of the 2D-Ising Model,” <http://quantumtheory.physik.unibas.ch/bruder/Semesterprojekte2007/p1/index.html> (2007).
 - ¹² L. Onsager, “Crystal Statistics. I. A Two-Dimensional Model with a Order-Disorder Transition,” *Phys. Rev.* **65**, 117 (1944).

Data for the critical exponents

		X_Max	mu_c	dX_Max	C_Max	FWHM[C]	dFWHM[C]
1,28	16x16	50,10286791	-1,893939394	20,3	40,04130981	0,1010101	0,025
1,29		49,9886915	-1,919191919	14	45,60287081	0,1010101	0,025
1,3		56,34934286	-1,919191919	19,2	41,38156039	0,1010101	0,025
1,31		52,24389222	-1,919191919	45	52,44868775	0,07575758	0,025
1,28	32x32	27,22660942	-1,893939394	9	43,45016951	0,07575758	0,025
1,29		35,69861266	-1,919191919	24	31,96171005	0,15151515	0,025
1,3		25,8301089	-1,919191919	9	29,70166616	0,1010101	0,025
1,31		29,74290147	-1,919191919	6	56,9692996	0,07575758	0,025
1,28	48x48	15,53856853	-1,893939394	5,5	36,08283846	0,07575758	0,025
1,29		25,19706822	-1,919191919	6,8	31,35591662	0,1010101	0,025
1,3		18,17688856	-1,893939394	4,8	42,71167422	0,07575758	0,025
1,31		22,70202687	-1,944444444	7,8	37,11128427	0,1010101	0,025
1,28	64x64	14,02544231	-1,944444444	2,4	19,74524386	0,17676768	0,025
1,29		14,03232228	-1,893939394	6,3	27,49778593	0,12626263	0,025
1,3		8,376392028	-1,944444444	2,7	18,52993825	0,2020202	0,025
1,31		13,35238913	-1,868686869	8	24,79823595	0,12626263	0,025

	1,28	1,29	1,3	1,31
gamma	1,822477659	0,731893518	0,460453234	-0,895583389
error(gamma)	3,797303442	16,56825195	3,520938341	11,99365604
rel_error(gamma)	208,36%	2263,75%	764,67%	1339,20%