Ageing at the Spin-Glass/Ferromagnet Transition: Monte Carlo Simulation using GPUs

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We study the non-equilibrium ageing behaviour of the $\pm J$ Edwards-Anderson model in three dimensions for samples of size up to $N = 128^3$ and for up to $10^8$ Monte Carlo sweeps. In particular we are interested in the change of the ageing when crossing from the spin-glass phase to the ferromagnetic phase. The necessary long simulation times are reached by employing a CUDA-based GPU implementation, which allows for single-spin flip times as small as 8ps. We measure typical spin glass correlation functions in space and time to determine the growing length scale and extract the constituting exponents. We observe a clear signature of the disorder-driven equilibrium transition in the non-equilibrium behavior.

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I. INTRODUCTION

Spin glasses are certain magnetic alloys that possess at low temperatures interesting equilibrium and non-equilibrium behaviour which is to a large extent still not well understood. The low-temperature ordered spin-glass phase is characterized by a rough free-energy landscape and by slow glassy dynamics. Disorder and frustration in the spin-spin interactions were identified as the underlying principals governing the behavior of spin glasses. Thus, models mixing positive, i.e., ferromagnetic and negative (antiferromagnetic) couplings such as the mean-field Sherrington-Kirkpatrick model and the Ising-like short-ranged Edwards-Anderson model were created to understand the spin-glass behavior. A prevailing topic is still, whether the replica-symmetry-breaking theory arising from the solution of the former model can accurately describe the spin-glass phase of the latter model in three dimensions. The most prominent competitor is the droplet theory, which centers around the eponymous droplets, low-level excitations from the presumably only two existing pure states. Numerous publications have dealt with simulations in as well as out of equilibrium.

The standard spin-glass models assume an on average equal fraction of positive and negative couplings. Nevertheless, when decreasing the fraction of negative bonds in the Edwards-Anderson model, it exhibits a phase transition at low temperatures from the aforementioned spin-glass phase to the well known ferromagnetic phase of the Ising model. This transition has been studied in the typical equilibrium approach to phase transitions also via ground-state calculations. Nevertheless, concerning the non-equilibrium “ageing” behavior, so far only systems deep in the spin-glass phase have been studied extensively, to the knowledge of the authors. Therefore, the purpose of this study is to determine, whether the spin-glass to ferromagnet transition is also visible within the non-equilibrium behaviour. Specifically we will be looking at growing correlations in space and time and try to explain them in terms of the dynamical correlation length. The determination and characterization of this growing length scale in the spin glass phase has been a focus of many previous publications, as there are a few stumbling blocks before dependably measuring it. It was quickly found, that it appears to follow a power law in line with the mean-field theory, though there is discussion whether it crosses over into the logarithmic growth expected from droplet theory.

Because reaching sufficiently long simulation times is computationally challenging, even inspiring the adoption of specialized hardware, we implemented the model in CUDA to leverage the comparatively high processing power of GPUs. Quite a few pioneering works have already tested the feasibility and performance outlook of this platform for the Ising and the Edwards-Anderson model but have shown no fruitful application. Our implementation has been carefully optimized for tackling the problem at hand efficiently and with limited resources. This allowed us to study large system sizes of $N = 128^3$ up to long time scales of $10^8$ sweeps.

The remainder of this work is organized as follows: In section we describe the used Edwards-Anderson model and its observables. Section follows with details on the GPU implementation of the model. The results of the simulation and their analysis are presented in section. We close with our conclusions in section.

II. MODEL

The Edwards-Anderson model describes a $D$-dimensional cubic system of side length $L$ containing $N = L^D$ Ising spins $S_i = \pm 1$. Its Hamiltonian is given by

$$H(S) = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j$$

(1)

where the sum runs over nearest neighbors $\langle i,j \rangle$ and the bonds $J_{ij} = \pm 1$ are drawn from a bimodal distribution $P(J) = p\delta(J - 1) + (1 - p)\delta(J + 1)$. We use periodic
of integral estimators for this problem. One uses the

\[ \xi_{18–20,24} \]

spin glass order parameter is the overlap

measured in sweeps) after the beginning of the simulation.

We then examine the system at different waiting times \( t_w \) (measured in sweeps) after the beginning of the simulation. The spin glass order parameter is the overlap

\[ q = \frac{1}{N} \sum_i q_i \quad (2) \]

with \( q_i = S_i^{(a)} S_i^{(b)} \) the element-wise overlap of two replicas \( S_i^{(a)} \) and \( S_i^{(b)} \) with the same bond configuration \( J \), but different initial configurations and thermal histories. In equilibrium, corresponding to \( t_w \rightarrow \infty \), the probability distribution \( P(q) \) is expected to assume a two peak structure below the transition temperature. In the droplet theory, this takes the form of two delta peaks at \( \pm q_{EA} \), while the mean-field theory has a wider distribution with a plateau of non-zero probability around \( q = 0 \).

To measure the growing length scale we make use of the spatial four-point correlation

\[ C_4(r, t_w) = \frac{1}{N} \sum_i q_i(t_w) q_{i+r}(t_w) \quad (3) \]

between two points and two replicas. With \( i + r \) we denote a spin which has a spacial distance \( r \) from spin \( i \).

There exist different approaches to extract a growing coherence (or dynamic correlation) length \( \xi \) from the four point-correlation function. The first approach is based on the assumption that \( C_4 \) follows the functional form

\[ C_4(r, t_w) \propto r^{-\alpha} g \left( \frac{r}{\xi(t_w)} \right) . \quad (4) \]

The function \( g \) is approximately a stretched exponential \( g(x) \sim \exp(-x^\beta) \). Extracting \( \xi \) works by fitting to the data of \( C_4 \), for various times \( t_w \). The two unknown exponents (\( \alpha \approx 0.5 \) and \( \beta \approx 1.5 \) in the spin-glass phase) complicate the extraction of \( \xi \), which spawned many methods for accomplishing this task.\cite{18, 20, 23}

As an alternative, notably Ref. 29 introduced the use of integral estimators for this problem. One uses the integral

\[ I_k(t_w) = \int_0^{L/2} r^k C_4(r, t_w) \ dr \quad (5) \]

to calculate an estimate for the coherence length

\[ \xi_k(t_w) = \frac{I_{k+1}(t_w)}{I_k(t_w)} \sim \xi(t_w) . \quad (6) \]

The choice of \( k \) determines which regions of the function \( C_4 \) contribute most to the estimate. Ref. 26 recommends \( k = 1 \) to get the best trade-off between systematic errors for small values of \( k \) and larger influence of statistical error for higher values.

Another observable of interest we use to study the aging behavior around the ferromagnet-spin glass transition is the autocorrelation

\[ C(t, t_w) = \frac{1}{N} \sum_i S_i(t_w) S_i(t_w + t) \quad (7) \]

between two points in time separated by a time difference \( t \) in reference to the waiting time \( t_w \). It is assumed to split into two parts. The first is a quasi-equilibrated part for small \( t \ll t_w \), that takes the form of a power law

\[ C_{eq}(t) \propto t^{-x} , \quad (8) \]

with another characteristic exponent \( x \). For longer times \( t \gg t_w \) the ageing part \( C_{age}(t, t_w) = f(\xi(t_w + t)/\xi(t_w)) \) can trivially be expected to depend only on the ratio of the coherence lengths at the two different times. An additive decomposition \( C(t, t_w) = C_{eq}(t) + C_{age}(t, t_w) \) is favored by theoretical arguments.\cite{18, 19, 21, 23, 27}. But we will make use of a multiplicative decomposition \( C(t, t_w) = C_{eq}(t) \cdot C_{age}(t, t_w) \), as this seems to work better, even though it is only expected to hold in the critical region.\cite{8, 23}

III. IMPLEMENTATION

We implemented a Metropolis Monte Carlo simulation\cite{30} of the model for Nvidia GPUs using the CUDA C programming interface, as was first detailed in Ref. 10. For explanation of the GPU-related terms used in the following we refer to the CUDA Programming Guide\cite{31} or a textbook like Ref. 11. In order to perform the update of a spin \( S_i \) one has to calculate the flipping probability

\[ p_{accept} = \min \left( 1, \exp \left( -\frac{2}{T} \sum_{j \in N(i)} J_{ij} S_i S_j \right) \right) \quad (9) \]

incorporating the coupling of the spin \( i \) to the local field generated by its direct neighbours \( N(i) \) on the lattice. Since GPUs are designed to keep their large number of simple processors busy with many, preferably independent processes at once, a sequential implementation of a single-spin-flip algorithm is ill-suited for GPUs. So in order to attain a parallel algorithm suitable for this architecture we adopted a standard checkerboard update scheme. In a first step all “white fields” of the system...
We choose spins from the same position in 64 different samples, which is sometimes known as asynchronous multispin-coding. Bit operations are used to perform the update for all bit-coded spins at the same time. We only need to differentiate between a few possible cases of spin alignments using boolean logic at the bit level. Then we look up the precalculated flipping probabilities from constant memory and apply them for the matching bits. It is customary to save computational effort by using only one random number for multiple samples. As no suitable and efficient random number generators were available at the time of implementation, we established a 1024bit variant of a Xorshift generator. The generator was optimized for generating a single random number per thread and kernel, as was needed here. With this complete implementation we reach single-spin-flip times of $\approx 8$ ps on a GeForce GTX 570 GPU. Of the prior implementations of Ising and Edwards-Anderson model only the one by Weigel is faster. But it uses multi-bit updates, which means each thread block updates for several flip-attempts per spin, thus requiring the costly global synchronization less frequently. This is no problem if one is interested in equilibrium properties, but this changes the dynamics, as, e.g., visible by the reduced growth of correlations. Therefore, that is undesirable when one wants to actually study the non-equilibrium dynamic ageing properties, as in the current work.

For the current work we only had access to two GPUs and consequently designed this approach for maximum efficiency per GPU. However if one had access to a larger number, it would be preferable to be able to distribute samples better among GPUs. For this purpose one can simply reduce the number of samples to $M = 2^m$ ($m < 6$) by storing $64/M$ spins from different positions per sample in a multispin. A simple way is to split the system into $64/M$ equal parts along one dimension and assign spins at the same relative positions to the bits $\{i, i + M, i + 2M, \ldots\}$ in the same multispin. This effectively makes it look and work like a smaller system with the caveat, that when coupling over the “periodic boundary” one has to rotate the bits of the multispin variable by $M$ positions. The computational overhead for this change is negligible but it has two other problems. Firstly this effectively shrinks our systems which might result in low occupancy and efficiency of the GPUs processors. But the bigger problem is, that we cannot use the same random number for spins from the same sample. Thus we have to generate $64/M$ random numbers per kernel instead of just one. Because of this requirement, the synchronous multispin-coding corresponding to $M = 1$ is very inefficient, and more balanced choice like $M = 8$ is preferable.

**IV. RESULTS**

We simulated a total of 192 samples of randomly initialized 128 systems with two replicas each. The sim-
FIG. 2. (Color online) Spatial correlation $C_4$ over the distance $r$ at different waiting times $t_w$ for a $128^3$ system at $p = 0.5$. Multiple close points were merged to give a clearer picture.

FIG. 3. Scaling exponent $\alpha$ of the spatial correlation over the bond probability $p$ for a $128^3$ system. The vertical line marks $p = p_c$. Inset: Associated scaling exponent $\beta$.

Our first approach to extracting this coherence length $\xi$ is a fit of $g$ with the stretched exponential form for $g$. However, the values $\alpha \approx 0.5$ and $\beta \approx 1.5$ which are suitable deep in the spin-glass phase ($p \approx 0.5$) might depend on the value of $p$. To get the most consistent values at a particular $p$ we performed multifits of the curves for all different $t_w \geq 10$ at once, i.e. with universal values of $\alpha$ and $\beta$ (independent of $t_w$), but individual values $\xi(t_w)$. Naturally the choice of points included in the fit can have an influence on the outcome. As such we generally restricted it to $r \geq 3$ and specifically found the cleanest results, when only using points at integer-valued distances $r$. Those are always located along the lattice axes. But as a reference we did the same fits also with all $r \geq 3$ and use these for calculating our errorbars for $\alpha$, $\beta$ and $\xi$. In detail we estimate our errors as the difference between the fit results for our restricted point set and the larger one plus both of the normal statistical errors from the two different fits. Still, this might underestimate the errors a bit, because for multifits statistical independence of the data is assumed, while in our case the measurements are from the same runs, just at different waiting times $t_w$, thus they are correlated.

The results for both exponents $\alpha$ and $\beta$ as a function of the probability $p$ are shown in Fig. 3. A strong change can be seen around the phase transition $p_c \approx 0.77$ from $0.4 < \alpha < 0.5$ and $1.4 < \beta < 1.45$ in the spin glass phase to $\alpha \approx 0$ and $\beta \approx 1.3$ in the ferromagnetic phase. Thus, the equilibrium phase disorder driven phase transition is well visible in the analysis of the non-equilibrium ageing behavior. Note that when getting closer to $p = 1$, i.e., in the ferromagnetic phase, the system quickly develops long-range order. Nevertheless, due to the low temperature, this is not an equilibrium magnetized configuration but a system with two large domains separated by a long-living domain wall. Thus, on the one hand, when addressing the range where the coherence length is small, we only have the first few time $t_w$ available to work with, i.e., the fits according to $g$ generally cannot be fitted as well at later times.

The second approach for calculating $\xi$ uses the integral estimation $\xi_t$ according to $h$. Like in the original work we take the integrals up to the point, where the value of $C_4$ first becomes smaller than three times its error, and approximate the rest of the integrals with our fitted function. Fig. 4 shows results for the coherence length $\xi$ as a function of the waiting time $t_w$ for both different approaches, respectively. As is visible from the figure, both methods agree well for a large stretch of waiting times but disagree close to the beginning and the end. While the integral results look closer to a power law, the fit results give a bit higher estimates for $\xi$ at the end and bend down at short times. A grave problem arises with finite size effects in the ferromagnetic phase, as can be seen in the inset of Fig. 4. When $\xi$ becomes comparable to the system’s own length scale $L$, the values get overestimated and the systems start to actually equilibrate. This means we would need to go to even larger systems.

Simulations were performed on two GeForce GTX 570. We took the parameters $T = 0.8$ and $p \in [0.5, 1]$ and performed $10^6$ time steps, which takes about 63h per batch of 64 multispin-coded samples. At the measure points the whole system configurations where simply stored to hard disk and the generated data was later post-processed to gain access to the correlation functions.

An exemplary spatial correlation $C_4$ from $h$ for $p = 0.5$ is shown in Fig. 3. The two replicas utilized for the calculation make correlations visible despite the model’s inherent disorder. The curves show a seemingly exponential decay for larger distances. The steeper gradient for small distances is incorporated in the scaling form $g$ with the power law $r^{-\alpha}$. As one would expect, the correlations spread to larger distances as time passes suggesting a growing length scale.
of ferromagnetic bonds, we fitted power laws of the form \( \xi(t_w) \sim t_w^{\beta} \), which is the most-simple yet widespread approach. This power-law behavior however is subdued at the beginning. So for fitting purposes we found, it is best to add a constant term, that then usually takes negative values. The determined exponents \( \beta \) for different \( p \) are shown in Fig. 5 for both methods of extracting \( \xi \). The vertical line marks \( p = p_c \).

Anyway, to study the dependence on the concentration \( p \) of ferromagnetic bonds, we fitted power laws of the form

\[
\xi(t_w) \sim t_w^{\beta} \quad \text{for} \quad L = 128^3 \quad \text{and} \quad L = 64.
\]

For \( L = 128 \), the two curves correspond to the fitting and integral estimation of \( \xi \) respectively, which agree pretty well. To give an impression of the finite-size effects, also the result from the fitting approach for \( L = 64 \) (exhibiting more systematic errors due to the small system size) is included.

The vertical line marks \( p = p_c \).

FIG. 6. (Color online) Autocorrelation \( C \) as a function of the time distance \( t \) at different waiting times \( t_w \) for a \( 128^3 \) system at \( p = 0.5 \).

Phase transition can again be seen. Starting from a constant value between 10 and 11 in the spin glass phase \( z \) has a peak around the phase transition before decreasing in the ferromagnetic phase. Larger values of \( z \) correspond to slower growth of correlations and consequently overall slower behaviour and equilibration. So it fits expectations that the spin glass phase has much higher values of \( z \) than the ferromagnetic phase. But interestingly we can see an even more pronounced slowdown in the critical region around the disorder-driven phase transition. Here the dynamics are so slow that one could expect even just a logarithmic growth of the coherence length with waiting time. Thus, we also tried right at \( p \approx p_c \) a fit to the functional form \( \xi(t_w) \sim \log(t_w/t_0)^{\tilde{z}} \) with parameters \( t_0 \) and \( \tilde{z} \). The fit worked as well as the power-law fit, thus, we are not able to distinguish a very slow power-law growth from a logarithmic growth here. For values of \( p \) close to one, note that the finite-size effect in \( \xi \) affects the values of \( z \), which causes a deviation from the expected \( z = 2 \) for \( p = 1.0 \). Furthermore, we tried to extrapolate the value of \( p_c \) from this data. For this purpose, we fitted a Gaussian to the peaks of the \( L = 64 \) and \( L = 128 \) data, while the data for \( L = 32 \) has a very pronounced peak at \( p = 0.78 \) (spacing \( \Delta p = 0.01 \)). As a result, we obtain estimates \( p_c(L = 32) = 0.78(1), \ p_c(L = 64) = 0.777(2) \) and \( p_c(L = 128) = 0.772(1) \). Thus, no pronounced finite-size effect is visible, see also the peak of the \( L = 64 \) data in Fig. 6. This can be expected, since we analyzed non-equilibrium data in the time interval where the coherence length is much smaller than the system size. Thus, it does not make much sense to try to extrapolate \( p_c \) for large system sizes, which appears anyway not necessary since the obtained values for \( p_c \) are very well compatible with the finite-size estimate from equilibrium studies.

In order to validate these results for \( \xi \) we will take a look at the autocorrelation \( C \) from Fig. 6. An example for \( p = 0.5 \) is shown in Fig. 6. Transitions can be seen...
around \( t = t_w \), respectively, from the equilibrium regime with slow algebraic decay to the ageing regime with faster decay. This corresponds to the notion that up to time \( t_w \) the system is equilibrated on length scales of size \( \xi(t_w) \) and it takes time \( t > t_w \) to make a spin feel that a system is not equilibrated at longer length scales.

To obtain the so-called equilibrium exponent \( x \) defined in \(^5\) we fit corresponding power laws to regions of different width, the smallest being \( t \in [100, t_w/1000] \). As the values agree well for the different fitting regions and \( t_w \), we take the mean as our result. We show in Fig. 7 the equilibrium exponent \( x \) at different probabilities. The exponent drops at the phase transition from a finite value \( x \approx 0.019 \) for the spin glass \( p = 0.5 \) to basically zero for the ferromagnet \( p = 1.0 \). This simply means that the equilibrium correlation in the ferromagnetic phase is not equilibrated at longer length scales.

Next we test the assumption, that the ageing part scales with \( \xi(t_w + t)/\xi(t_w) \) by trying a collapse in Fig. 8 using a multiplicative decomposition \( C(t_w,t) = C_{eq}(t) \cdot C_{age}(t_w,t) \). We used the results for \( \xi \) previously obtained using the fit approach. This gave a better collapse than the integral results especially for small \( t_w \). For the display in Fig. 8 we subtract 1 from our abscissa to make the collapse of values for \( t \ll t_w \) and thus \( \xi(t_w + t) \approx \xi(t_w) \) better visible. As visible from the figure, the quality of the collapse is very good. The optimal value of \( x \approx 0.016 \) for the collapse is a bit smaller than the fit result shown in Fig. 7 and generally seems to be susceptible to the particular form of \( \xi \). Note that we tried also collapses with an additive decomposition \( C(t_w,t) = C_{eq}(t) + C_{age}(t_w,t) \) but this resulted for all cases in a worse overlap of the curves even with its additional free parameter.

V. CONCLUSION

We were able to perform relatively long simulations of the Edwards-Anderson model at low temperatures for multiple different probabilities from the spin glass phase up to the ferromagnetic one. This was made possible largely through the use of general-purpose GPU (CUDA) computing, which has become feasible in recent years. Thus, the CUDA-based approach allows for very fast simulations of spin glasses at much cheaper costs compared to standard CPU systems or even compared to specific FPGA-based hardware like the Janus computer.\(^{30}\)

The ageing behavior of the spin glass phase seen in previous study was reproduced well. The main purpose of our work was to study the ageing behavior of the system as a function of the variable fraction of ferromagnetic bounds. We could easily detect the transition from the spin-glass phase to the ferromagnet, when altering the bond probability \( p \). This was visible in all quantities we measured. Note that only at the extreme end of the ferromagnetic phase finite size effects began to complicate matters considerably and we cannot give exact results there. Our entry point, the spatial correlation, contains information about the growing length scale of a system but, because we lack an explicit form for it, getting reliable values is difficult. The integral estimators taken from Ref. 26 and 29 have proven useful but do not seem to work as well at short times. A multifit of the assumed form \(^\) can help out for these cases. It also turns out the matching form changes noticeably when crossing the phase transition line. While the exponent \( \beta \) of the stretched exponential only lowers slightly, the other exponent \( \alpha \) basically vanishes in the ferromagnetic phase, thus arriving at a simpler form.

The autocorrelation exhibits a quasi-equilibrated part with power law behavior in the spin-glass phase. The
equilibrium exponent $x$ also vanishes in the ferromagnetic phase, which does not exhibit as much rearrangement in equilibrium. The ageing part on the other hand can be scaled well with the quotient $\xi(t_w+t)/\xi(t_w)$, also giving credence to their calculated values. The assumption of power law growth works for the coherence length albeit with a small correction for early values. However we did not delve into testing a crossover to logarithmic growth. The power law exponent $z$ is naturally higher for the slower dynamics of the spin glass. But it also shows additional slowdown in the critical region around the phase transition. In essence all findings agree with the general expectations that in the ferromagnet the equilibrium state is more uniform and stationary and systems can arrive there much faster. Nevertheless, we were quite surprised how well the equilibrium disorder-driven transition shows up when measuring the non-equilibrium ageing properties.

However our whole approach was focused on the long time simulation of spin glasses and as such we could not get as good results for the ferromagnet. Because of the faster evolution a different emphasis would have to be put to fare better. Also it can be seen as a bit questionable to make use of the trick of recycling random numbers for different samples without a strong influence of the disorder. In any case, beyond the physical results, the developed implementation and analysis methods can be used to proceed further efficiently with investigations of the equilibrium and non-equilibrium behavior of the random bond model.

VI. ACKNOWLEDGMENTS

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