Bona Fide Thermodynamic Temperature in Nonequilibrium Kinetic Ising Models

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We show that a nominal temperature can be consistently and uniquely defined everywhere in the phase diagram of large classes of nonequilibrium kinetic Ising spin models. In addition, we confirm the recent proposal that, at critical points, the large-time “fluctuation-dissipation ratio” $X_\infty$ is a universal amplitude ratio and find in particular $X_\infty \approx 0.33(2)$ and $X_\infty = \frac{1}{2}$ for the magnetization in, respectively, the two-dimensional Ising and voter universality classes.

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The fluctuation-dissipation theorem (FDT), which relates the correlation and response (or susceptibility) functions during the return to equilibrium following a small perturbation, may be used to provide an absolute definition of the temperature of a physical system. However, there are many instances, such as glassy materials and coarsening systems, where the standard form of the FDT breaks down, because the equilibration timescales are astronomical or even infinite in the thermodynamic limit. Relaxation properties then depend upon both $t$ and $t'$, at which perturbations are applied. In this context, guided by the dynamics of some mean-field spin glass models, Cugliandolo and Kurchan [1] have proposed a generalized form of the FDT:

$$R(t, t') = \frac{X(t, t')}{T} \frac{\partial C(t, t')}{\partial t}, \quad (1)$$

where the two-time response and auto-correlation functions $R(t, t')$ and $C(t, t')$ of some physical observable, as well as the so-called FDT ratio $X(t, t')$, are not functions of $t' - t$ and, moreover, $X$ depends functionally on $C$. The limit value $X_\infty$, often taken by $X$ at large times is usually interpreted as the emergence of an “effective temperature” $T_{\text{eff}} = T/X_\infty$ [2].

The picture suggested by the above generalized FDT scenario has received a large number of confirmations [3], both from experimental [4] and numerical [5, 6, 7] studies of structural and spin glasses, granular matter, and gently sheared fluids, to quote a few examples. In these situations, the physical systems under consideration, though they may never achieve equilibration, evolve subject to a temperature $T$. However, this “nominal” temperature is generally not even defined for intrinsically nonequilibrium systems, e.g. stochastic models for which detailed balance is violated, although such systems are known to behave much like their equilibrium counterparts, including critical behavior and non-stationary properties of their two-time autocorrelation and response functions.

In this Letter, we show that a nominal temperature can be consistently and uniquely defined everywhere in the phase diagram of large classes of nonequilibrium kinetic Ising models. We explain how both a “dynamical” definition of temperature (using Eq. (1)) and a “geometrical” approach (in terms of the density of states) lead to an ambiguity that can be lifted using a maximum-entropy argument. This results in a unique, bona fide thermodynamic temperature which takes the same value for different observables and coincides with the usual one when detailed balance is satisfied. In addition, considering the critical points of our models, we confirm the proposal [8, 9] that $X_\infty$ is, in this context, a universal amplitude ratio of dynamic scaling functions and find in particular $X_\infty[M] \approx 0.33(2)$ and $X_\infty[M] = \frac{1}{2}$ for the magnetization $M$ in, respectively, the two-dimensional Ising and voter [10] universality classes.

For simplicity, we illustrate our approach by considering the family of two-dimensional nonequilibrium kinetic spin models introduced some time ago in [11] which are defined by the following evolution rules. During an elementary timestep, an Ising-like spin $(\sigma_x = \pm 1)$ on a square lattice is randomly picked up, and flipped with a probability $W[E_r = -\frac{1}{2}\sigma_r H_r]$ where $E_r \in \{-2, -1, 0, 1, 2\}$ is the local (pseudo-)energy, $H_r = \sum_{\mu=i,j} \sigma_{1+r_\mu}$, being the local (Weiss-like) field calculated over the four nearest neighbors of $\sigma_r$. The local $Z_2$-symmetry of the dynamical rules is enforced by demanding that $W(-E) = 1 - W(E)$ (the system being homogeneous, we drop spatial indexes whenever possible) and thus $W(0) = \frac{1}{2}$, leaving a two-parameter family defined by $W(1) = \frac{1}{2}(1+x)$ and $W(2) = \frac{1}{2}(1+y)$, with $-\infty < x < y < 1$. An alternative convenient parameterization [12] is to match the flip rate $W$ with the corresponding expression for Glauber dynamics ($W = \frac{1}{2}(1 + \tanh 2\beta E)\cos\theta$ at temperature $T = \frac{1}{\beta}$). This is only possible if one introduces two parameters $\beta_1 \equiv \beta_{E=1}$ and $\beta_2 \equiv \beta_{E=2}$, such that $x = \tanh 2\beta_1$ and $y = \tanh 4\beta_2$, which measure respectively the strength of interfacial and bulk noise [13]. The usual Glauber dynamics then corresponds to $\beta_1 = \beta_2 = 1/T$, or, equivalently, $y = 2x/(1 + x^2)$. Other well-studied models in the $(x, y)$-plane comprise the majority model ($y = x$), the “noisy voter” or linear model ($y = 2x$), and the “extreme” model ($x = 1$). Except on the Glauber line, mod-
els in the \((x, y)\)-plane do not obey detailed balance or possess an underlying short-range Hamiltonian. Nevertheless, in agreement with a long-lasting conjecture backed up by field-theoretic arguments \[12\] \[16\], there exists a critical line \(y_c(x)\) separating a disordered (paramagnetic) from an ordered (ferromagnetic) phase and along which Ising static and dynamic critical exponents are numerically found (Fig. 1) \[11, 12, 13\]. This line terminates at the voter model critical point \((\frac{1}{2}, 1)\), across which the transition occurs in the absence of bulk noise \((y = 1)\) \[10\].

The gist of our argument to define an effective temperature is the observation that, even if the FDT may be broken at large times, there always exists, for small time-differences \((t' - t \leq \mathcal{O}(1))\) and \(t \gg 1\), an equilibrium-like regime where the standard form \([11\) is valid with \(X = 1\). Thus, in this two-time sector, and in particular for \(t' - t \ll 1\), we view \(\beta_{\text{dyn}}\) as a means of obtaining a dynamical definition of an effective temperature \([1\] : 

\[
\frac{1}{T_{\text{dyn}}} \equiv \lim_{t \to \infty, t' \to t} \frac{R(t, t')}{\partial_t C(t, t')}.
\] (2)

To really make sense of \([2]\), we must of course specify the response function \(R(t, t')\), i.e. we have to implement, for a generic \((x, y)\)-model, a definition of a symmetry-breaking external field \(h\), linearly conjugated to the local spin variable \(\sigma_x\). Probably the simplest choice is to make the substitution \(\sigma_x H_r \to \sigma_x (H_r + h_r)\) in the original expression of \(W_r\), this simple recipe also being consistent with the natural redefinition \(E_r \to E_r^{(h)} = E_r - \sigma_r h_r\) of the energy in this case. This yields:

\[
W_r^{(h)} = \frac{1}{2} (1 - \sigma_r \tanh \beta_{\text{dyn}} (H_r + h_r)).
\] (3)

The problem we face now is that an extra parameter \(\beta_0\) appears, which governs the fate, under the influence of the applied field \(h_r\), of configurations where \(H_r = 0\). One might think that the arbitrariness in the choice of \(\beta_0\) for a generic \((x, y)\)-model could be resolved by demanding that \(\beta_{\text{dyn}}\) would give the same effective temperature for all observables. This is not the case: in fact, general properties of the spin-flip dynamics we consider automatically guarantee that, for any given value of \(\beta_0\), our definition \([2]\) of \(\beta_{\text{dyn}} = 1/T_{\text{dyn}}\) does not depend on the observable chosen to evaluate the corresponding correlation and response functions since it can be re-expressed as

\[
\beta_{\text{dyn}} = \frac{\langle \sigma \partial h W_r^{(h)} \rangle_{h=0}}{\langle W_r \rangle} = \frac{\langle 2 \beta_{\text{dyn}} E_r (1 - W_r) \rangle}{\langle W_r \rangle},
\] (4)

where the average is over all lattice sites \([13\).

The way out of this quandary is deceptively simple: as for the Glauber model, where \(\beta_0\) is of course equal to the inverse of the true temperature, one has to tune \(\beta_0\) such that any FDT measurement with a probing field yields precisely \(\beta_0\) as the effective temperature. That is to say, for any \((x, y)\)-model, \(\beta_0\) is the solution of

\[
\beta_{\text{dyn}}(\beta_0) = \beta_0.
\] (5)

Because \(\beta_0\) only appears, in Eqs. \([2\) - \([1]\), in the initial condition \(R(t, t^+)\) of the response function \([13\), the dependence of \(\beta_{\text{dyn}}\) on \(\beta_0\) is simply linear, and the solution of \([5]\) is therefore unique.

The reason why Eq. \([5]\) is the correct prescription is a profound, geometric one, and is incidentally the same as for the Glauber model: this choice of \(\beta_0\) actually maximizes the entropy of the spin configurations. To understand this point, recall that at equilibrium the canonical Botzmann-Gibbs distribution can also be obtained from the microcanonical ensemble under an information-theoretic, maximum-entropy condition \([21\), where the Lagrange multiplier \(\beta_{\text{geo}}\) (identified with the inverse temperature in units where \(k_B = 1\)) imposing the mean value of the energy reweights with an exponential prefactor \(\propto e^{\beta_{\text{geo}} E}\) the bare probabilities of the spin configurations. Then, for any \((x, y)\)-model on a finite system a steady-state is always attained, and it is perfectly legitimate to define a microcanonical entropy \(S_{\text{mic}}(M, E) \equiv \ln \Omega(M, E)\) where the density of states \(\Omega(M, E)\) simply counts the number of configurations having a prescribed magnetization \(M\) and energy \(E\) as reached by the spin-flip dynamics. But in this "microcanonical" ensemble, the only spin-flip allowed are those which do not change the energy, that is the ones corresponding to \(W(0) = \frac{1}{2}\), a value common to all \((x, y)\)-models. In other words, the
influence of distinct \((x, y)\)-values can only be felt if one lets the energy fluctuates, in which case — and for exactly the same reasons as above — one should expect to actually observe the configurations with an effective reweighting \(\propto e^{\beta_\text{geo} E}\), leading to a “canonical” entropy \(S_{\text{can}}\). Now, if one works with a non-zero external field \(h\) in the microcanonical ensemble (in particular around the most probable values of \(M\) and \(E\)), to lowest-order in \(h\), once again, only the spin-flips with \(H_r = 0\) will be allowed, with a probability \(\hat{\Omega}(E)\) which can be rewritten as \(W(h)(0) = \frac{1}{\beta_\text{geo} E^{h/2}}\). This expression shows that a consistent reweighting can be achieved if and only if \(\beta_\text{geo} = \beta_0\), an equality that \(\ref{eq:1}\) also recovers if one restricts the average to zero local-field configurations.

To check the validity of the above scenario, we have computed the density of states (reweighted) using an efficient algorithm \(\ref{eq:2}\) which allows to determine, with high accuracy, the ratios \(\frac{\hat{\Omega}(M, E')e^{\beta_0(E'-E)}}{\hat{\Omega}(M, E)}\) for neighboring (i.e. connected by a single spin-flip) magnetization and energy levels. This method is applicable anywhere in the \((x, y)\)-plane, except of course for \(y = 1, 1/2 \leq x \leq 1\) when no fluctuations are present. It produces, in particular, fast and accurate estimates by restricting the calculations to a narrow interval centered around the stationary (and most probable) values \(M_{\text{sta}}\) and \(E_{\text{sta}}\), with or without an external field. The above ratios also provide a direct access to an estimate of \(\frac{\partial S_{\text{can}}(M, h\beta_0)}{\partial M}\) which — if the above effective thermodynamic picture is valid — should be equal to \(h\beta_\text{geo}\) in the disordered phase (where for any system size \(M_{\text{sta}} = 0\)). This is indeed verified for sufficiently small \(h\) and, most importantly, it is only so when one has tuned \(\beta_0\) according to \(\ref{eq:1}\) (Fig. 2a).

In the ordered phase or along the critical line, finite-size fluctuations of the energy bring in another term (stemming from the differentiation of \(e^{\beta_\text{geo} E}\) in the effective occupation probabilities) which cannot be evaluated simply with the present method. But one can nevertheless have an indirect access to the dependence of the absolute entropy on \(\beta_0\) by working, with and without magnetic field, along the magnetization direction in an interval comprising both \(M_{\text{sta}}\) and \(M_{\text{sta}}\), because this last quantity depends on \(\beta_0\). In particular, if the selected value of \(\beta_0\) is the extremalizing one, the difference \(\delta S(M) = \frac{\partial S_{\text{can}}(M, E, h\beta_0)}{\partial M} - \frac{\partial S_{\text{can}}(M, E, 0)}{\partial M}\) should be as flat as possible. This is confirmed in Fig. 2b for the critical point of the majority model.

To sum up, our nominal temperature is unique and can be determined in two equivalent ways for any \((x, y)\) model (see Fig. 1b for an example). We note in passing that two models sharing the same stationary energy (e.g. Glauber and linear for which this quantity is known exactly \(\ref{eq:3}\)) are usually not at the same effective temperature. Of particular interest is the non-monotonous variation of the temperature \(T_c\) along the critical line (Fig. 1c). Once \(T_c\) determined, one can study the long-time behavior of \(X\). Using a now-standard method \(\ref{eq:4}\), the parametric representation of Fig. 3a yields the universal limit \(\chi_\infty = 0.33(2)\). This value while in disagreement with \(\ref{eq:5}\), has also been obtained independently in \(\ref{eq:6}\) and \(\ref{eq:7}\), and is consistent with the two-loop RG results of \(\ref{eq:8}\).

Further (analytical) insight can be gained for the linear and critical voter model: along the line \(y = 2x\), all correlation functions do not couple to higher-order ones, and verify diffusion equations. Using standard Laplace-Fourier methods much as for the Glauber 1d-Ising chain, one can not only calculate exactly the stationary energy, but also obtain many exact results for the correlation and response functions. Skipping all technical details \(\ref{eq:9}\), the two-time two-point correlation function \(C_t(t', t) = \langle \sigma(t)\sigma(t') \rangle\), is compactly expressed in terms of a double Laplace transform \(\tilde{C}_t(s, s') = \frac{1}{sq_0(s/2)}\frac{\hat{\delta}(s/2)}{s'-s/2}\) \((s \leftrightarrow s, s' \leftrightarrow t)\), where \(q_t(t) = e^{-\beta_0 q_0(2xt)}\), \(p_t(t)\) being the probability that a simple random walk goes from 0 to \(x\) during a length of time \(t\) \((p_0(t) = e^{-\beta_0 t^2/2})\) \(\approx 1/(\pi t)\), where \(I_0\) is a modified Bessel function. Specializing to the autocorrelation function \(C(t, t') = \tilde{C}_t(t, t')\), this gives for \(x < 1/2\) when \(t\) is large and \(t' - t\) arbitrary \(C(t, t') \approx 1 - \int_t^{t'-t} du q_0(u)/q_0(0)\), a function of \(t' - t\) decaying exponentially on a timescale \(\tau_x = 1/(1 - 2x)\). At the voter critical point, both \(q_0(0)\) and \(\tau_x\) diverge, and the previous expression crosses over to a non-trivial two-time scaling form, with \(C(t, t') \approx 1 - (\ln t)^{-1} t'^-t\) \(du q_0(u)\) in the first temporal regime \(t'/t \gg 1\), \(t' - t \sim O(1)\) which matches at large time differences the result \(C(t, t') = (\ln t)^{-1}\ln(\frac{t'}{t})\) valid in the second regime \(t'/t \gg 1\). As for the autoresponse function \(R(t, t')\) it simply reads \(R(t, t') = q_0(t' - t)R(t' - t)\). For \(x < 1/2\), \(R(t, t')\) tends to a finite and non-zero constant, and an effective FDT is obeyed at all times, with \(X(t, t') = 1\). For the voter model, \(R(t, t') \approx (\pi/\ln t)|\beta_0 - \beta_0|\) in the long-time limit, where the numerical constant \(c_4\)
is such that $\langle \prod_{\mu=1}^{4} \sigma_\mu(t) \rangle \simeq 1 - c_4 \pi/\ln t$. Hence (11) reads $\beta_{\text{dyn}}(\beta_0) = \beta_0 - \frac{3}{4}(\beta_0 - \beta_1)c_4$, and the prescription (8) is realized when $\beta_0 = \beta_1$, thus bypassing the evaluation of (5). The time $t_c$ is easily measured for both $M$ and $E$ and found equal to the exact value above (Fig. 3b), the long-time regime is difficult to reach numerically. For the magnetization, we find $X_\infty[M] = 0.50(5)$ (not shown), which gives an indication of the accuracy of the Ising value above. For the energy, however, the signal is too weak to estimate $X_\infty[E]$ so that we cannot test the conjecture (24) that $X_\infty$ is the same for all observables, which seems unlikely to us given that critical static amplitudes ratios usually depend on the observable considered.

Summarizing, we have shown how to measure the “strength of noise” via a bona fide thermodynamic temperature in kinetic spin models and confirmed the universality of the FDT ratio $X_\infty$ at critical points. Ongoing work aims at extending our method to even more general nonequilibrium systems such as chaotic map lattices.

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[1] L. F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. 71, 173 (1993); J. Phys. A 27, 5749 (1994).
[2] L. F. Cugliandolo, J. Kurchan, and L. Peliti, Phys. Rev. E 55, 3898 (1997).
[3] For a recent review, see: L. F. Cugliandolo, Les Houches July 2002 Lecture Notes [cond-mat/0210312].
[4] T. S. Grigera and N. E. Izraelev, Phys. Rev. Lett. 83, 5038 (1999); L. Bellon, S. Ciliberto, and C. Laroche, Europhys. Lett. 53, 511 (2000); D. Héricher and M. Ocio, Phys. Rev. Lett. 88, 257202 (2002).
[5] G. Parisi, Phys. Rev. Lett. 79, 3660 (1997); J.-L. Barrat and W. Kob, Europhys. Lett. 46, 637 (1999).
[6] A. Barrat et al., Phys. Rev. Lett. 85, 5034 (2000); H. Makse and J. Kurchan, Nature 415, 614 (2002).
[7] L. Berthier, J.-L. Barrat, and J. Kurchan, Phys. Rev. E 61, 5464 (2000); L. Berthier and J.-L. Barrat, J. Chem. Phys. 116, 6228 (2002).
[8] C. Godrèche and J.-M. Luck, J. Phys. A 33, 1151 (2000).
[9] C. Godrèche and J.-M. Luck, J. Phys. A 33, 9141 (2000).
[10] I. Dornic, H. Chaté, J. Chave, and H. Hinrichsen, Phys. Rev. Lett. 87, 045701 (2001).
[11] M.J. de Oliveira, J. F. F. Mendes and M. A. Santos, J. Phys. A 26, 2317 (1993).
[12] J.-M. Drouffe and C. Godrèche, J. Phys. A 32, 249 (1999).
[13] J. F. F. Mendes and M. A. Santos, Phys. Rev. E 57, 108 (1998); T. Tomé and M. J. de Oliveira, Phys. Rev. E 58, 4242 (1998).
[14] Two-temperature models (e.g. one for spin-flips and one for spin-exchanges) have been studied, but attempts at defining an effective temperature have been largely unsuccessful. See, e.g.: P. L. Garrido, J. Marro, and J. M. Gonzalez-Miranda, Phys. Rev. A 40, 5802 (1989); M.A. Santos and S. Teixeira, J. Stat. Phys. 78, 963 (1995).
[15] G. Grinstein, C. Jayaprakash, and Y. He, Phys. Rev. Lett. 55, 2572 (1985).
[16] K. E. Bassler and B. Schmittmann, Phys. Rev. Lett. 73, 3343 (1994); U. C. Täuber, V. K. Akkineni, and J. E. Santos, Phys. Rev. Lett. 88, 045702 (2002).
[17] The limit $t \to \infty$ is somewhat formal: after some microscopic time $\tau_0$ becomes actually time-independent.
[18] The proof is easy, if formal. For instance, if $C_M(t,t') = \langle \sigma_{t'}|\sigma_t \rangle$ is the autocorrelation of the (local) magnetization, and $C_O(t,t') = \langle O_n(t)|O_n(t') \rangle$ that of an observable $O_n = \prod_{k=1}^{n} \sigma_{t_k}$ then $\partial_{t'} C_M(t,t') = \sum_{\sigma_{t'}}\langle O_n(t)|O_n(t')W_{\sigma_{t'}}(t') \rangle$ tends to $-\sum_{\sigma_{t}}\langle W_{\sigma_{t}}(t) \rangle n\partial_t C_M(t,t') \color{red}{\Lbrace_{t=t'} \to t^+}}$ (due to the continuity of the master equation, $\sigma_{t'}(t) = 1$ and translation invariance). Similarly, the corresponding response functions are related by $R_M(t,t') = nR_M(t,t')$, and the factor $n$ thus cancels when calculating the ratio appearing in (24).
[19] Explicitly, this initial condition (of e.g. the magnetization) reads $R_M(t,t') = \frac{\beta(t) - 1 - \tanh^2\beta(t)}{\beta(t)}$, which expression was naturally understood once developed on the “basis” of correlation functions involving all possible products of the 4 neighbors $\{\sigma_{t+\epsilon_\mu}\}_{\mu=1,...,4}$ of a given spin. One finds $R_M(t,t') = r_0 + r_1 \sum_{\mu} \langle \sigma_{t+\epsilon_\mu}(t)|\sigma_{t+\epsilon_\mu}(t') \rangle + r_2 \sum_{\mu,\nu} \langle \sigma_{t+\epsilon_\mu}(t)|\sigma_{t+\epsilon_\mu}(t') \rangle$, with e.g. $r_0 = \frac{2}{3} - \frac{1}{3} + \frac{1}{3} \tau_0(1 - \tanh^2\beta(t)) + \beta_1(1 - \tanh^2\beta(t))$.
[20] E. T. Jaynes, Phys. Rev. 106, 620 (1957).
[21] A. H"uller and M. Pleimling, Int. J. Mod. Phys. C 13, 947 (2002) [cond-mat/0110900].
[22] F. Sastre, I. Dornic, and H. Chaté, in preparation.
[23] A. Barrat, Phys. Rev. E 57, 3629 (1998).
[24] P. Mayer, L. Berthier, J. P. Garrahan, and P. Sollich, Phys. Rev. E 68, 016116 (2003).
[25] C. Chatelain, cond-mat/0303452 (v2 of 21 July 2003).
[26] P. Calabrese and A. Gamba, Phys. Rev. E 65, 066120 (2002); 66, 066101 (2002).
[27] These equalities are valid in any space dimension, so that...
$X_\infty = \frac{1}{2}$ for the voter class as defined in [10].