Measurement-Noise Maximum as a Signature of a Phase Transition

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We propose that a maximum in measurement noise can be used as a signature of a phase transition. As an example, we study the energy and magnetization noise spectra associated with first- and second-order phase transitions by using Monte Carlo simulations of the Ising model and 5-state Potts model in two dimensions. For a finite size system, the total noise power and the low frequency white noise $S(f < f_{\rm knee})$ increase as T_c is approached. In the thermodynamic limit, $S(f < f_{\rm knee})$ diverges but $f_{\rm knee} \to 0$ and the total noise power vanishes. $f_{\rm knee}^{-1}$ is approximately the equilibration time.

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Noise is ubiquitous and is being increasingly used as an experimental tool to probe condensed matter systems, but unfortunately, when studying phase transitions, the usefulness of the experimental results is diminished by the fact that little is known about what to expect in the noise spectra. We propose that an increase in the measurement noise can be used to signal the onset of a phase transition since noise arises from the fluctuations of microscopic entities which, in turn, play a key role in phase transitions. For example, as a second-order phase transition is approached, thermal fluctuations are associated with a growing correlation length that characterizes the size of the fluctuating entities and with such things as critical opalescence in binary fluids [1]. These growing fluctuations should produce an increase in the noise power as the transition is approached. In general, it is plausible that a maximum in the noise in any quantity that is produced by microscopic fluctuations should signal a phase transition. Past studies indicate that resistance noise increases in the vicinity of the metal-insulator transition [2], a spin glass transition [3], and phase transitions of molecules adsorbed onto metallic carbon nanotubes [4]. Using noise to look for a phase transition could be especially useful in systems such as driven systems [5] or granular systems [6] where thermodynamic and transport measurements are problematic. However, there are competing tendencies. In the thermodynamic limit, growing fluctuations lead to divergences in quantities such as the susceptibility and the specific heat, but the noise in measurements goes to zero due to self-averaging.

As a simple test case, we have done a systematic study to determine if the noise power increases in the vicinity of well-understood first- and second-order phase transitions. We use Monte Carlo simulations to study the noise spectra of the energy and magnetization per spin associated with the phase transitions in two models. In the thermodynamic limit the 2D Ising model has a second-order phase transition marked by divergences in the specific heat C_V and magnetic susceptibility χ at the transition temperature $T_c = 2.269$ [7], while the 2D 5-state Potts model has a weakly first-order phase transition marked by delta function singularities in C_V [8] and χ [9] at $T_c = 0.85$ [10]. The temperature is in units of J/k_B, where we set the ferromagnetic exchange $J = 1$ and k_B is the Boltzmann constant. C_V and χ are proportional to the variance σ^2 of the energy and magnetization fluctuations, respectively. Correspondingly, we find that, for a given number of spins N, the total noise power per time step, $S_{\rm tot}$, as well as the low frequency noise $S(f < f_{\rm knee})$ increase as the transition temperature is approached. Here f is the frequency and $f_{\rm knee}$ is a crossover frequency. At T_c, $S(f < f_{\rm knee})$ is independent of frequency and diverges in the thermodynamic limit, but $f_{\rm knee}$ and $S_{\rm tot}$ vanish as $N \to \infty$. $f_{\rm knee}^{-1}$ is approximately equal to the minimum sampling time $\Delta t_{\rm eq}$ needed to obtain accurate thermodynamic averages. For the Ising model $f_{\rm knee}$ scales like the relaxation rate τ^{-1}. At high frequencies we find for both models that the noise spectral density $S(f > f_{\rm knee})$ goes as $1/f^{\mu}$, where the exponent $\mu < 2$. In the case of the second-order phase transition, we can relate the exponent μ to the critical exponents by using the fluctuation-dissipation theorem and the theory of dynamic critical phenomena. Our relation for μ confirms previous theoretical work which used noise spectra to obtain critical exponents for the 2D Ising model [11,12].

The Hamiltonians of the 2D Ising model and the 2D 5-state Potts model are $H_{\rm Ising} = -J\sum_{i<j} s_i s_j$ and $H_{\rm Potts} = -J\sum_{i<j}\delta(s_i, s_j)$, respectively, where $\delta(x, y)$ is the Kronecker delta function and (i, j) denotes the nearest neighbor sites on a square lattice. The spins can take values $s_i = \pm 1$ for the Ising model and $s_i = 0, 1, 2, 3, 4$ for the Potts model. For both models, we apply periodic boundary conditions for different system sizes $N = L \times L$, where $L = 10, 20, 40, 80, 160$. We use Metropolis Monte Carlo simulations to obtain the time series of the energy and magnetization. In each simulation, we start from a high temperature ($T = 10$), and then gradually cool the system to $T = 0.5$. Starting from either hot or cold initial temperatures has little effect on the noise. At each temperature, we wait until the system equilibrates before recording the time series that consists of the energy and magnetization

per spin for at least $10 \times 2^{17} = 1,310,720$ Monte Carlo time steps per spin (MCS). The specific heat per spin $C_V = N\sigma_E^2/k_B T^2$ and the susceptibility per spin $\chi = N\sigma_M^2/k_B T$ are calculated from σ_E^2 the variance of the energy per spin and from σ_M^2 the variance of the magnetization per spin.

We define the equilibration time Δt_{eq} of the energy (magnetization) to be the minimum sampling time needed to obtain an accurate thermodynamic average of the energy (magnetization). To determine Δt_{eq}, we use a block averaging technique [13,14] in which we divide the energy (magnetization) time series into equal segments of length Δt, calculate the specific heat (susceptibility) from the fluctuations in each segment, and then average these values. The average C_V (χ) and σ_E^2 (σ_M^2) initially increase as Δt increases, and then plateau at the equilibrium value when $\Delta t \geq \Delta t_{eq}$.

The amplitude of the energy and magnetization fluctuations is largest at T_c as shown in Fig. 1 for the 2D Ising model. This is reflected in the distributions of the energy and the magnetization which are much wider at T_c than at

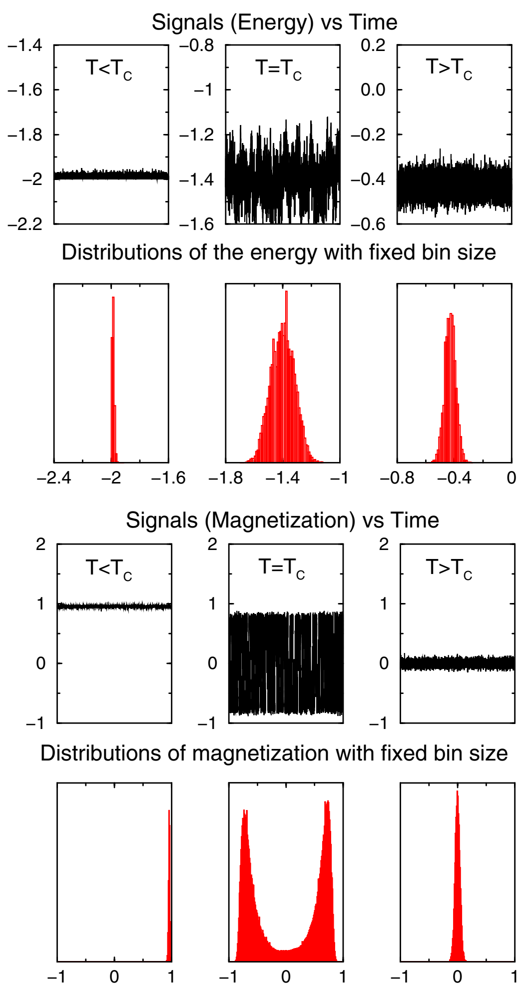

FIG. 1 (color online). Time series (with 10^4 MCS) and distributions of the energy and magnetization for the 2D Ising model ($L = 40$) at different temperatures. Energy and magnetization distributions are from a run with 10^4 and 10^6 MCS, respectively.

other temperatures. This is also true for the 5-state Potts model. Thus, the larger the variance, the longer it will take to fully sample the energy and magnetization distributions at the critical temperature, and the larger Δt_{eq} will be. We shall see that as a result f_{knee} in the noise spectrum will shift to lower frequencies. The increase in the noise and the variances at the critical temperature are consistent with the peaks in C_V and χ vs T in finite size systems.

Next we calculate the noise spectral density. From the Wiener-Khintchine theorem, the spectral density $S_x(f)$ of a time series $x(t)$ is proportional to the Fourier transform of the autocorrelation function $\Psi_x(t)$ of the fluctuations $\delta x(t) = [x(t) - \langle x \rangle]$: $S_x(f) = 2\int dt e^{i2\pi f t}\Psi_x(t)$. We choose the normalization so that the total noise power per time step is

$$S_{tot} = \frac{1}{N_\tau}\sum_{f=0}^{f_{max}} S_x(f) = \sigma_x^2, \quad (1)$$

where N_τ is the length of the time series and σ_x^2 is the variance of $x(t)$. This way, for a stationary signal $x(t)$ with power law correlations, $S_x(f)$ will be approximately the same for different signal lengths. Notice that S_{tot} will be largest at T_c for a given N.

The noise spectral densities are shown in Fig. 2. At low frequencies, the noise power $S(f)$ is largest at T_c. In the high ($T \to \infty$) and low ($T \to 0$) temperature limits, the noise power is small and white noise. At intermediate temperatures, the noise spectra have a plateau at low frequencies and scale as $1/f^\mu$ at high frequencies, where the exponent $\mu < 2$. We denote the crossover frequency between these two regimes by f_{knee}.

For the 2D Ising model the exponent μ at T_c can be related to the critical exponents by using the fluctuation-dissipation theorem and dynamic critical phenomena [15]. The frequency-dependent susceptibility $\chi(\omega)$, where $\omega = 2\pi f$, scales as $\chi(\omega) \sim \varepsilon^{-\gamma}\hat{\chi}(x)$, where $\hat{\chi}$ is a scaling function, $x = \omega\tau \sim \omega/\varepsilon^{z\nu}$, z is the dynamic critical exponent associated with the relaxation time $\tau \sim \xi^z$, ν is the critical exponent associated with the divergence of the correlation length $\xi \sim \varepsilon^{-\nu}$, γ is the critical exponent associated with the divergence of the magnetic susceptibility $\chi \sim \varepsilon^{-\gamma}$, and $\varepsilon = |(T/T_c) - 1|$ is the reduced temperature. As $x \to \infty$,

$$\chi(\omega) \sim \varepsilon^{-\gamma}\left(\frac{\omega}{\varepsilon^{z\nu}}\right)^{-a}. \quad (2)$$

At T_c, ε must disappear from $\chi(\omega)$. So $a = \gamma/z\nu$ and $\mathrm{Re}\chi(\omega) \sim \omega^{-\gamma/z\nu}$. Since $\chi(t)$ is real, $\mathrm{Re}\chi(\omega) = \mathrm{Re}\chi(-\omega)$, and from the Kramers-Kronig relation we find

$$\mathrm{Im}\,\chi(\omega) = \frac{1}{\pi}P\int_{-\infty}^{+\infty}\frac{\mathrm{Re}\chi(\omega')}{\omega - \omega'}d\omega' \sim \omega^{-\gamma/z\nu}, \quad (3)$$

for all $\omega > 0$, where P denotes the Cauchy principal value. Thus from the fluctuation-dissipation theorem, the power spectrum of the noise becomes

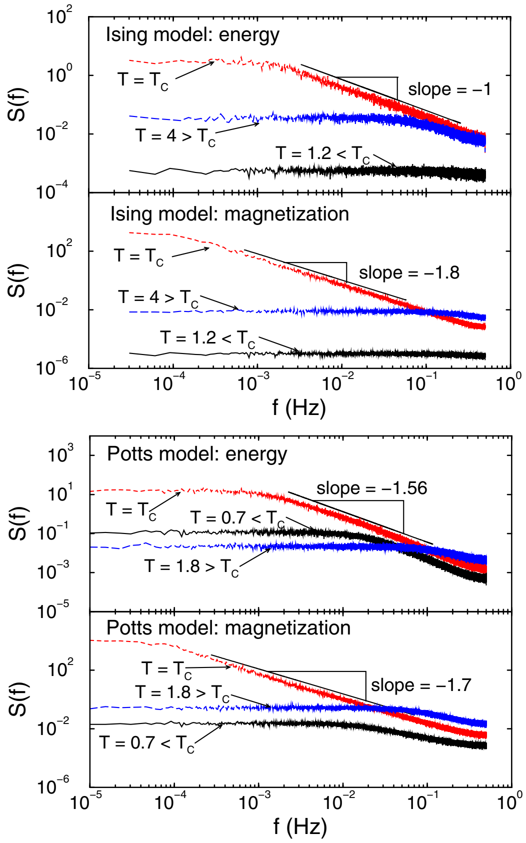

FIG. 2 (color online). Noise spectra of the energy and magnetization fluctuations for the 2D Ising model ($L = 40$, 1 run per temperature) and the 2D 5-state Potts model ($L = 10$, 4 runs per temperature). The exponent $\mu = -$slope.

$$S_M(\omega) = \frac{4k_BT}{\omega}\,\mathrm{Im}\chi(\omega) \sim \omega^{-1-(\gamma/z\nu)}, \qquad \forall\ \omega > 0. \quad (4)$$

So for the magnetization $\mu_M = 1 + (\gamma/z\nu)$. For the 2D Ising model, where $\nu = 1$, $\gamma = 7/4$ [7], and $z = 2.17$ [16], we find $S_M(f) \sim f^{-1.81}$. From the Monte Carlo simulation shown in Fig. 2, $S_M(f) \sim f^{-1.8}$, which agrees very well with our analytic result. Similarly, for the energy noise of the 2D Ising model, $\mu_E = 1 + (\alpha/z\nu)$ where we now use the specific heat exponent $\alpha = 0$ [7] instead of γ. We find $\mu_E = 1$, i.e., $1/f$ noise ($S_E(f) \sim f^{-1}$) for $f \gg f_{\mathrm{knee}}$, and this agrees with Fig. 2. Our expressions for μ_M and μ_E agree with those from [11,12], though they derived them differently. For the 5-state Potts model, since it has a first-order phase transition, there are no critical exponents, so the above arguments do not apply.

We now consider f_{knee}, which marks the transition from white noise to power law behavior. The characteristic time scale $\tau_{\mathrm{knee}} = 1/f_{\mathrm{knee}}$ is set by the equilibration time Δt_{eq}. Figure 3 shows the noise spectra and the block scaling results as a function of $1/f$ or Δt. We see that the time scale $1/f_{\mathrm{knee}}$ where the power spectrum $S(f)$ flattens off is comparable to the time Δt_{eq}. Since the variance is constant for $\Delta t > \Delta t_{\mathrm{eq}}$, $S(f)$ will be constant for $f < f_{\mathrm{knee}}$ [13].

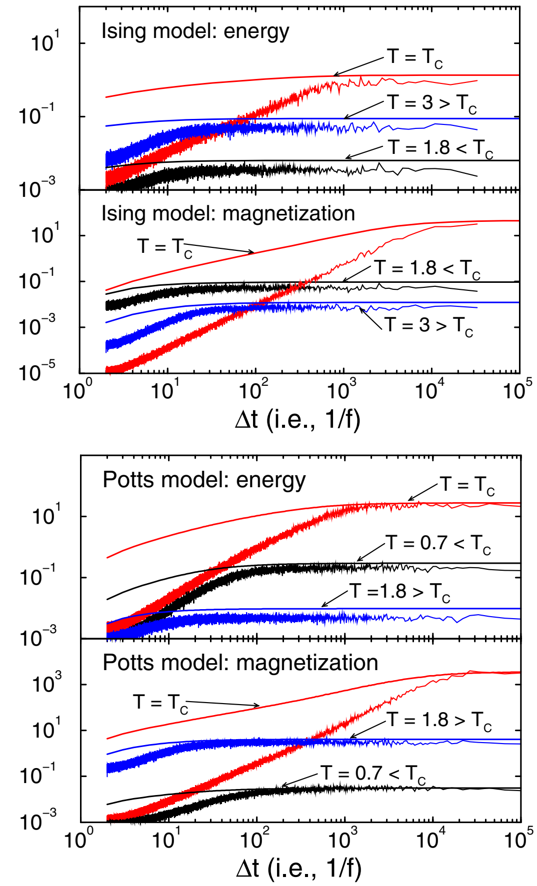

FIG. 3 (color online). Comparison of the block scaling of C_V (for the energy) and χ (for the magnetization) with the noise spectra. Thick smooth solid line: C_V (or χ) vs block size Δt. Thin noisy solid line: power spectrum of the energy (or magnetization) vs $1/f$, which is equivalent to block size Δt. Ising data are from 1 run per temperature, and Potts data are from 5 runs per temperature. All signals have been vertically shifted for better viewing.

Since Δt_{eq} has a maximum at T_c, f_{knee} is a minimum at T_c and increases as T moves away from T_c.

For the 2D Ising model in the critical region, we expect $1/f_{\mathrm{knee}}$ to scale in the same way as the relaxation time τ [17]:

$$f_{\mathrm{knee}}^{-1} \sim \tau \sim L^z\hat{\tau}(L/\xi) \sim L^z\hat{\tau}[L^{1/\nu}(T - T_c)]. \quad (5)$$

This scaling gives good agreement with our results as shown in Fig. 4 where we plot $1/(L^z f_{\mathrm{knee}})$ vs $L^{1/\nu}(T - T_c)$. So for the 2D Ising model, $f_{\mathrm{knee}} \sim 1/L^z \sim 1/N^{z/d}$, where d is the dimension. Using $\nu = 1$, we find that the best fit for the dynamical scaling exponent is $z = 2.1 \pm 0.2$, which is consistent with previous results [11,12,16]. For the 2D 5-state Potts model, scaling with τ does not apply, but $f_{\mathrm{knee}} \sim 1/N \sim 1/L^d$.

Size dependence.—In general, we expect the energy and magnetization per spin in larger systems to be self-averaging, and hence to have smaller fluctuations and less noise. For the models we studied, at T_c, $S(f) \sim 1/(Nf^{\mu})$ at

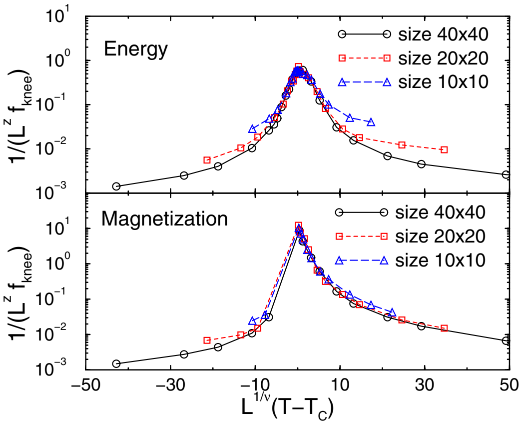

FIG. 4 (color online). Scaling of the knee frequency $f_{\rm knee}$ at temperatures close to T_c for the 2D Ising model. Setting $\nu = 1$, we find that $z = 2.1 \pm 0.2$ gives a universal scaling function at $T \approx T_c$.

high frequencies ($f > f_{\rm knee}$), and $S(f) \sim S(f_{\rm low}) \sim 1/(N f_{\rm knee}^{\mu})$ at low frequencies ($f < f_{\rm knee}$). Since $f_{\rm knee} \sim N^{-b}$, where $b = 1$ for the 2D 5-state Potts model and $b = z/d$ for the 2D Ising model, in the thermodynamic limit the low frequency noise diverges at T_c: $S(f_{\rm low}) \sim N^{b\mu - 1} \rightarrow \infty$ as $N \rightarrow \infty$ if $\mu > 1/b$ [11]. $\mu > 1/b$ for the energy and magnetization spectra of both models, so $S(f_{\rm low})$ diverges. However, this low frequency region disappears in the thermodynamic limit: $f < f_{\rm knee} \sim N^{-b} \rightarrow 0$ as $N \rightarrow \infty$ since $b > 0$. [At $f = 0$, $S(f = 0) = 0$.] As $N \rightarrow \infty$, $S_{\rm tot}$ is finite and decreases as $N^{b(\mu-1)-1}$ with increasing system size.

We now turn to the size dependence at temperatures far away from T_c where our simulations show that $S(f) \sim 1/N$ and that $f_{\rm knee}$ is the same for different N. Our simulations verify that the variances decrease as the temperature goes away from T_c. Moreover, at very high and very low temperatures, our simulations agree with the analytic result that the variances per spin go as $1/N$. In particular, when $T \rightarrow \infty$, the spins are uniformly distributed, and one can show analytically that for the 2D Ising model $(\sigma_E^2)_\infty = 2/N$ and $(\sigma_M^2)_\infty = 1/N$, while for the 2D q-state Potts model $(\sigma_E^2)_\infty = n(q-1)/(2q^2 N)$ and $(\sigma_M^2)_\infty = (q^2-1)/(12N)$, where n is the number of nearest neighbors. If, on the other hand, the temperature is close to zero so that the whole system experiences at most one spin flip after one MCS, the energy and magnetization obey a Poisson distribution, and the probability p of a spin flip goes as $p \sim N$. In this case, the variance per spin $\sigma_T^2 \sim p/N^2 \sim 1/N$ holds for both the energy and the magnetization of both models. The combination of $\sigma^2 \propto 1/N$ and Eq. (1) implies that at temperatures far away from T_c, $S_{\rm tot} \sim 1/N \sim 1/L^d$, which is confirmed by our simulations.

For time series of finite length in finite size systems in the temperature range $T^* < T < T_c$ where T^* is slightly below T_c, there can be large changes in the magnetization corresponding to large clusters of spins flipping. This can complicate the dynamics by increasing the variance of the magnetization. However, when $N \rightarrow \infty$, $T^* \rightarrow T_c$.

In summary, for fixed N, we show that fluctuations produce an increase in the low frequency noise $S(f < f_{\rm knee})$ and the total noise power $S_{\rm tot}$ as first- and second-order phase transitions are approached. For a given length of the time series, $f_{\rm knee}$ may be too low to observe if the system is too big, indicating that this approach to finding phase transitions is better suited to small systems. Even though the 5-state Potts model has a weakly first-order transition, we find very similar results for the 10-state Potts model which has a strong first-order phase transition. Our results show that a maximum in the low frequency noise as well as in the total noise power per time step can signal a phase transition. However, one complication is the presence of disorder, which can lead to an inhomogeneous transition, e.g., a transition occurring at slightly different temperatures in different parts of the sample. As a result, there may not be a clear signature of the transition in the noise [18]. However, if the noise does exhibit a maximum, then this is a good indication of a phase transition.

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