

## Collective excitations and retarded interactions

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We study the dynamics of many-body systems with retarded interactions and show how their non-Markovian character can lead to nonergodic behavior. This nonergodicity is characterized by the appearance of long periods or chaotic wanderings in phase space. We construct the phase diagrams for Ising-type systems with delayed interactions, and show the emergence of non-Gibbsian measures as a function of both interaction strengths and delays.

The dynamics of many-body systems has traditionally been considered in a framework where retardation effects play an insignificant role. Since for Coulomb interactions this approximation seems to work well, the results obtained by using either Boltzmann equations or master equations are considered to be an accurate representation of the time evolution of real systems. There are, however, problems where interactions are mediated through slower fields, such as phonons and magnons, and where these delays can play a significant role. This is, for example, the case of systems such as plastic crystals, superionic conductors, and ferroelectrics. In all these situations, the coupling between pseudospin degrees of freedom and phonon fields leads to anomalous phenomena in their critical dynamics, and a strong renormalization of the excitation spectra.<sup>1</sup> Moreover, the dynamics of many other diverse systems such as neural nets and computing structures<sup>2</sup> makes it necessary to include the effect of retardation in their asymptotic dynamical behavior.

It has recently been shown that in the limit of large delays such as those encountered in computer simulations of many-body systems, the appearance of discrete dynamics can have a profound influence on the asymptotic dynamics of statistical-mechanics systems.<sup>3</sup> In particular, the time evolution of such systems can be strongly nonergodic, leading to either very long cycles or chaotic wandering of expectation values. Since natural systems are bound to lie in between the extremes of negligible delays and large retardations, the question arises as to the role played by retarded interactions in determining the excitation spectra of many-body systems.

This paper reports results of a first attempt at addressing this issue in analytic fashion. We first consider the dynamics of a spin system where interactions can be mediated with arbitrary delays and show the non-Markovian nature of the resulting master equation. We next solve the dynamics of an Ising model in the one-dimensional case and obtain explicit formulas for the time evolution of observables as a function of the interaction delays. We then treat the higher dimensional case using local-field corrections to mean-field theory, and show how the interplay between delays and interaction strengths can

lead to nonergodic behavior. Finally, we construct a phase diagram displaying these features and provide some conjectures as to the existence of chaotic regimes in the asymptotic dynamics of the system. We believe that our results are of relevance to a number of statistical-mechanics systems, as well as providing analytic bounds for the breakdown of ergodicity as a result of retardation.

We consider a system of  $N$  sites the states of which are represented by binary variables  $s_i = \pm 1$  ( $i = 1, 2, \dots, N$ ). The state of the whole system can then be characterized by the  $N$ -tuple number  $(s_1, s_2, \dots, s_N) \equiv \alpha$ . Each site interacts with its neighboring sites and makes transitions between the two states according to conditional probabilities that depend on the states of neighboring sites as well as on the influence of an external world. If the interaction between sites is instantaneous, the conditional probabilities of the individual sites depend on the momentary states of neighboring sites (but not on the past states). The time evolution of the system can then be described by a Markov process in which the system has no memory except for its immediate past.<sup>4</sup>

In the more realistic case of retarded interactions, however, the individual sites see the past states of neighboring sites. This in turn leads to a non-Markov process in which the system does have memory. To describe it we introduce the conditional probability

$$p(\beta, t + \Delta t \mid \alpha, t; \alpha_1, t - \tau_1; \alpha_2, t - \tau_2; \dots; \alpha_n, t - \tau_n)$$

for the system to be in state  $\beta \equiv (s_1^{(\beta)}, s_2^{(\beta)}, \dots, s_N^{(\beta)})$  at time  $t + \Delta t$  given that it is in state  $\alpha$  at time  $t$  and in states  $\alpha_1, \alpha_2, \dots, \alpha_n$  at corresponding times  $t - \tau_1, t - \tau_2, \dots, t - \tau_n$  ( $0 \leq \tau_1 \leq \tau_2 \leq \dots \leq \tau_n$ ).

It is straightforward to derive a non-Markov master equation for the joint probability

$$P(\alpha, t; \alpha_1, t - \tau_1; \alpha_2, t - \tau_2; \dots; \alpha_n, t - \tau_n)$$

of the system being in state  $\alpha$  at time  $t$  and in states  $\alpha_1, \alpha_2, \dots, \alpha_n$  at corresponding times  $t - \tau_1, t - \tau_2, \dots, t - \tau_n$ :

$$\begin{aligned}
& P(\alpha, t + \Delta t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) - P(\alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) \\
&= - \sum_{\beta} [p(\beta, t + \Delta T | \alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) P(\alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) \\
&\quad - p(\alpha, t + \Delta t | \beta, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) P(\beta, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n)] . \quad (1)
\end{aligned}$$

This formulation has some similarity to that of Van Hove's,<sup>5</sup> where quantum interference results in a non-Markovian process which is negligible in the weak perturbation limit. We should remark, however, that in our case the non-Markovian character of Eq. (1) results from the retardation effect in interactions, an effect which is purely classical. Multiplying Eq. (1) by  $s_k$  and summing over  $\alpha, \alpha_1, \dots, \alpha_n$  we obtain the equation for the average value,

$$\begin{aligned}
\langle s_k \rangle_t &\equiv \sum_{\alpha} \sum_{\alpha_1} \dots \sum_{\alpha_n} s_k P(\alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) , \\
\langle s_k \rangle_{t+\Delta t} - \langle s_k \rangle_t &= -2 \sum_{\alpha} \sum_{\alpha_1} \dots \sum_{\alpha_n} s_k \sum_{\beta} p(\beta, t + \Delta t | \alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) P(\alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) , \quad (2)
\end{aligned}$$

where the prime in the summation over  $\beta$  implies the restriction  $s_k^{(\beta)} = -s_k$ .

We now assume that the conditional probability of the whole system can be expressed as a product of the conditional probabilities of the individual sites

$$p(\beta, t + \Delta t | \alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) = \prod_{i=1}^N p(s_i^{(\beta)}, t + \Delta t | s_i, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) , \quad (3)$$

an assumption which can be shown to be correct for the kinetic Ising model with retarded interactions. Equation (3) allows Eq. (2) to take the simple "single-spin-flip" form

$$\langle s_k \rangle_{t+\Delta t} - \langle s_k \rangle_t = -2 \sum_{\alpha} \sum_{\alpha_1} \dots \sum_{\alpha_n} s_k p(-s_k, t + \Delta t | s_k, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) P(\alpha, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) , \quad (4)$$

where we used the fact that

$$\sum_{s_i^{(\beta)}} p(s_i^{(\beta)}, t + \Delta t | s_i, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) = 1 . \quad (5)$$

We further assume that each site can change its own state instantaneously, and that the golden rule holds, which allows us to write the conditional probability in the form ( $\Delta t \rightarrow 0$ )

$$p(-s_k, t + \Delta t | s_k, t; \alpha_1, t - \tau_1; \dots; \alpha_n, t - \tau_n) = w_k(s_k; \alpha_1; \dots; \alpha_n) \Delta t , \quad (6)$$

where  $w_k(s_k; \alpha_1; \dots; \alpha_n)$  is the transition rate. Equation (4) then becomes

$$\frac{d}{dt} \langle s_k \rangle_t = -2 \langle s_k w_k(s_k; \alpha_1; \alpha_2; \dots; \alpha_n) \rangle_{t, t-\tau_1, \dots, t-\tau_n} , \quad (7)$$

where it is understood that the time arguments of the averages of  $\alpha, \alpha_1, \dots, \alpha_n$  are  $t, t - \tau_1, \dots, t - \tau_n$ , respectively. We thus obtain a difference-differential equation with time lags  $\tau_1, \tau_2, \dots, \tau_n$ .

We can similarly obtain the equations for correlation functions, which will not be attempted here. We should also note that it is straightforward to derive the linear-response theory for this system, which turns out to be entirely similar to that for systems with instantaneous interactions.<sup>6</sup>

As an example, we will now consider the kinetic Ising model with retarded interactions, whose energy is given by

$$E(\alpha; \alpha') = - \sum_{i,j} J_{ij} s_i s_j' - H \sum_{i=1}^N s_i , \quad (8)$$

where  $\alpha' \equiv \{s_i'\}$  is the configuration of the system at time earlier than the time of the configuration  $\alpha \equiv \{s_i\}$  by  $\tau$ . We will also consider the case of nearest-neighbor interactions, and retain just one time lag  $\tau = d/v$ , where  $d$  is the

distance between nearest neighbors and  $v$  is the propagation speed of interactions. In true equilibrium, the state of the system does not obviously change with time, and Eq. (8) becomes identical to the Hamiltonian of the ordinary Ising model. To describe the time evolution of the system, however, we need to consider the nonequilibrium situation in which the state changes with time.

We choose the transition rate as ( $\beta \equiv 1/k_B T$ )

$$w_k(s_k; \alpha') = \frac{1}{2\epsilon} [1 - s_k \tanh(\beta E_k')] , \quad (9)$$

where  $\epsilon$  is the relaxation time of a single spin in the presence of a heat bath, and  $E_k'$  is defined to be

$$E_k' \equiv \sum_l J_{kl} s_l' + H . \quad (10)$$

If we use Eqs. (3), (5), and (6), it is straightforward to show that the choice given by Eq. (9) satisfies the principle of detailed balance. Equation (9) then allows one to

write Eq. (7) in the form

$$\epsilon \frac{d}{dt} \langle s_k \rangle_t = -\langle s_k \rangle_t + \langle \tanh(\beta E_k) \rangle_{t-\tau}, \quad (11)$$

where time arguments are shown explicitly. In the limit of zero delay ( $\tau \rightarrow 0$ , instantaneous interactions), Eq. (11) becomes the continuous dynamics form—an ordinary differential equation—familiar in studies of the kinetic Ising model with instantaneous interactions,<sup>7</sup> i.e.,

$$\epsilon \frac{d}{dt} \langle s_k \rangle_t = -\langle s_k \rangle_t + \langle \tanh(\beta E_k) \rangle_t. \quad (12)$$

In the case of retarded interactions ( $\tau \neq 0$ ), we rewrite Eq. (11) in the dimensionless form

$$\frac{d}{dt} \langle s_k \rangle_t = -a \langle s_k \rangle_t + a \langle \tanh(\beta E_k) \rangle_{t-1}, \quad (13)$$

where  $t$  has been rescaled in units of  $\tau$ , and  $a \equiv \tau/\epsilon$  determines the dynamic processes of the system. The formal integration of Eq. (13) then leads to the integral equation

$$\langle s_k \rangle_t = a \int_{-\infty}^t e^{-a(t-t')} \langle \tanh(\beta E_k) \rangle_{t'-1} dt', \quad (14)$$

which, in the limit of infinite delays ( $\tau \rightarrow \infty$  or  $a \rightarrow \infty$ ) takes the digital dynamics form<sup>3</sup>

$$\langle s_k \rangle_t = \langle \tanh(\beta E_k) \rangle_{t-1}. \quad (15)$$

Equation (13) is known to have a unique solution for  $t > 1$  if the initial condition is given in the form<sup>8</sup>

$$\langle s_k \rangle_t = \phi_k(t), \quad 0 \leq t \leq 1. \quad (16)$$

We first consider a one-dimensional ring in the absence of external fields with  $J_{ij} = J$  for nearest neighbors. Equation (13) then becomes linear and takes the form with  $x_k(t) \equiv \langle s_k \rangle_t$  [ $\gamma \equiv \tan(2\beta J)$ ]

$$\dot{x}_k(t) = -ax_k(t) + \frac{1}{2}\gamma a [x_{k-1}(t-1) + x_{k+1}(t-1)] \quad (17)$$

or

$$\dot{\mathbf{x}}(t) + a\mathbf{x}(t) - \frac{1}{2}\gamma a\mathbf{B}\mathbf{x}(t-1) = \mathbf{0}, \quad (18)$$

where  $\mathbf{x}(t)$  is the column vector consisting of  $x_k(t)$ , and  $\mathbf{B}$  is a ("cyclic") matrix given by

$$\mathbf{B} = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & & & & \ddots & & & \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}.$$

The solution of Eq. (18) with the initial condition  $\mathbf{x}(t) = \phi(t)$ ,  $0 \leq t \leq 1$  can be expressed as a series

$$\mathbf{x}(t) = \sum_{n=1}^{\infty} e^{z_n t} \mathbf{p}_n(t), \quad t > 1 \quad (19)$$

where  $e^{z_n t} \mathbf{p}_n(t)$  is just the residue of  $e^{zt} H^{-1}(z) \mathbf{p}(z)$  at a zero  $z_n$  of  $\det \mathbf{H}(z)$ , and the vector  $\mathbf{p}(z)$  and the matrix  $\mathbf{H}(z)$  are given by

$$\mathbf{p}(z) = \phi(0) + \int_0^1 [\phi'(t) + a\phi(t')] e^{-zt'} dt', \quad (20)$$

$$H(z) = (z+a)\mathbb{1} - \frac{\gamma a}{2} e^{-z\mathbf{B}},$$

respectively. The explicit computation of  $z_n$ 's, the zeros of  $\det \mathbf{H}(z)$ , is complicated and will not be attempted in this paper. If the system is translationally invariant, however, i.e.,  $x_k(t) = x(t)$ , Eq. (19) takes the explicit scalar form

$$x(t) = \sum_{n=1}^{\infty} e^{z_n t} \frac{\phi(0) + \int_0^1 [\phi'(t') + a\phi(t')] e^{-z't'} dt'}{1 + \gamma a e^{-z_n}}, \quad (21)$$

where  $z_n$ 's are zeros of  $h(z) \equiv z + a - \gamma a e^{-z}$ . These zeros, which can be computed numerically for given  $a$  and  $\gamma$ , asymptotically take the form

$$z_n = -\ln \frac{(2n - \frac{1}{2} \operatorname{sgn} \gamma) \pi}{|\gamma a|} \pm i(2n - \frac{1}{2} \operatorname{sgn} \gamma) \pi + O\left(\frac{\ln n}{n}\right). \quad (22)$$

Since all zeros of  $h(z)$  have negative real parts for  $\gamma \neq 1$ ,<sup>9</sup> (i.e., at finite temperatures)  $x(t)$  as given by Eq. (21) decays to zero as  $t$  increases. This is to be expected since the two limiting cases [ $\tau \rightarrow 0$ , continuous dynamics given by Eq. (12) and  $\tau \rightarrow \infty$ , digital dynamics given by Eq. (15)] in one dimension display the same asymptotic behavior at finite temperatures. In fact, it has been shown that for sufficiently small delays, the solutions of difference-differential equations have the same asymptotic behavior as those of corresponding ordinary differential equations ( $\tau = 0$ ).<sup>10</sup>

In order to treat higher-dimensional systems we use a mean-field approximation together with local-field corrections. As with the corresponding case for digital dynamics,<sup>3</sup> we obtain Eq. (13) in the approximate form

$$\dot{x}(t) = -ax(t) + f[x(t-1)] \quad (23)$$

with

$$f(x) = a \tanh\{[J - (J')^2]x + (J')^2 x^3\}$$

where  $J \equiv \beta \sum_j J_{ij}$  and  $(J')^2 \equiv \beta^2 \sum_j J_{ij}^2$  are assumed to be the same for all sites. If the solution of the linearized equation of Eq. (23) around  $x = 0$  approaches zero as  $t$  increases, which is the case for

$$(J')^2 - |\operatorname{sech} p| < J < (J')^2 + 1 \quad (24)$$

with  $p$  given by the equation

$$p = -a \tanh p, \quad \frac{\pi}{2} \leq p < \pi \quad (25)$$

then the zero solution of Eq. (23) is also asymptotically stable<sup>8</sup> (see Fig. 1). If, however, Eq. (24) is not satisfied, the zero solution can be unstable, which is both the most interesting and the poorly understood case. In that case it is possible for a nonzero constant solution of Eq. (23) to

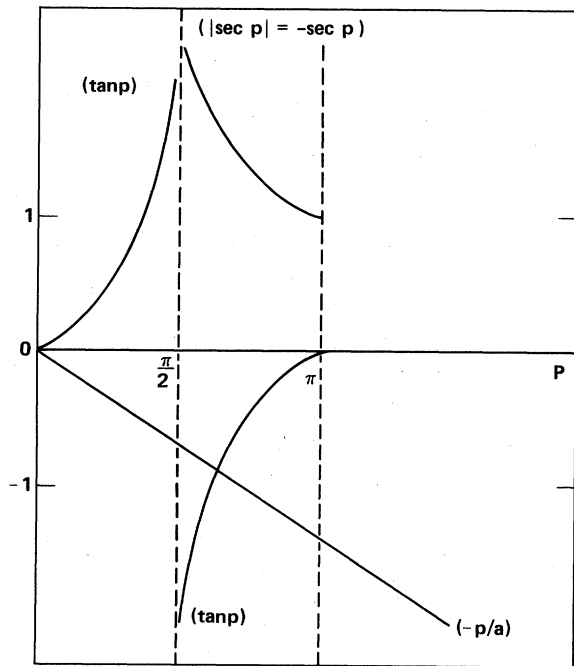


FIG. 1. Graphical solution of Eq. (25), displaying the behavior of the functions  $\tan p$  and  $\sec p$ .

become asymptotically stable. The corresponding condition can be obtained in a manner similar to Eq. (24). For some ranges of parameters  $a$ ,  $J$ , and  $J'^2$ , however, the solution of Eq. (23) can display periodic behavior. If the linearized equation is unstable, i.e., Eq. (24) is not satisfied, and in addition,  $J < 0$ , then Eq. (23) has a (nonconstant) periodic solution. Furthermore, it can be shown that the periodic solution is asymptotically stable if  $f(x)$  is monotone decreasing,<sup>11</sup> i.e.,  $J < -2J'^2$ .

If  $f(x)$  has both a decreasing part and an increasing part, which would be the case for  $-2J'^2 < J < J'^2$ , and the constant solution is still unstable, then it is likely that the solution will display even more complicated behavior. Though there does not exist a complete analysis for this "mixed-feedback" case, an der Heiden, Walther, and Mackey have shown the existence of chaotic behavior for a rather particular type of  $f(x)$ , and conjectured the existence of similar behavior for a larger class of  $f(x)$  as delay increases from 0 to  $\infty$ .<sup>12</sup> This conjecture has been indeed supported by several numerical experiments.<sup>13</sup> Therefore, it is very likely that Eq. (23) will display chaotic behavior as  $\tau$  increases since the corresponding difference equation ( $\tau \rightarrow \infty$  limit) has been shown to exhibit such behavior.<sup>3</sup> This expectation leads to the phase diagram shown in Fig. 2.

In conclusion, we have used joint probabilities to write a non-Markovian master equation for many-body systems with retarded interactions. The derived equations take the form of difference-differential equations similar to those studied in the literature.<sup>12,14</sup> It should be emphasized, however, that our formulation takes explicitly into account the interaction between the elements of many-body

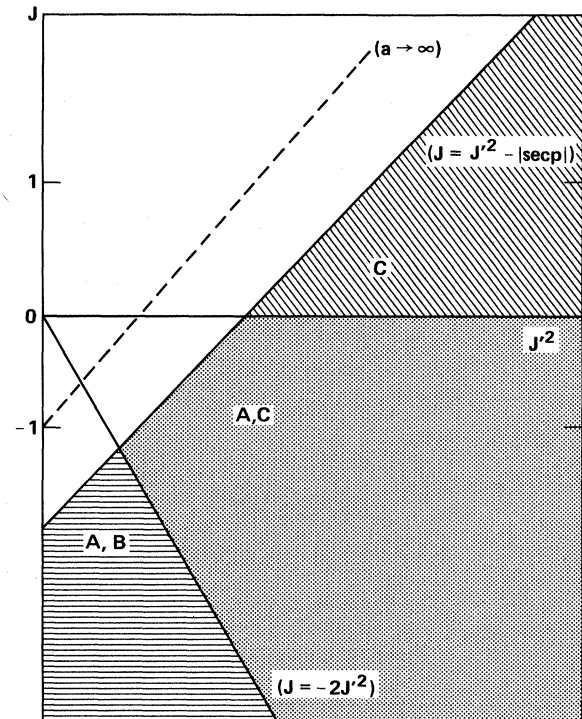


FIG. 2. Phase diagram of an Ising-type system with competing interactions as a function of interaction strength and delay times. Phase  $A$  denotes a periodic solution which may or may not be stable,  $B$  is the stable periodic solution, and  $C$  is the chaotic asymptotic phase.

systems, and therefore describes cooperative phenomena. We have also applied this formalism to the kinetic Ising model with retarded interaction, and obtained exact solutions to the dynamics in one dimension, which, at finite temperature decay to zero as time increases. In higher dimensions we have used the mean-field theory together with local-field corrections to obtain an approximate equation of motion, which can have a periodic solution. The explicit condition for the existence and stability of this periodic solution was also obtained. This regime is in sharp contrast to the ordinary differential equation which results from the kinetic Ising model with instantaneous interaction. We therefore conclude that systems with retarded interactions can exhibit behavior which is qualitatively different from that exhibited by systems with instantaneous interaction. This theory interpolates smoothly between the continuous dynamics and digital dynamics. From the standpoint of applications, this formalism will be relevant to any many-body systems in which the delay in the propagation is comparable to the relaxation time of the single element. This is the case for many systems, which appear in physics, biology, and geology such as superionic conductors,<sup>1</sup> neural networks,<sup>2</sup> propagation of disease, and fault systems.<sup>15</sup>

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