Relaxation in kinetic models on alternating linear chains

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A restricted dynamics, previously introduced in a kinetic model for relaxation phenomena in linear polymer chains, is used to study the dynamic critical exponent of one-dimensional Ising models. Both an alternating isotopic chain and an alternating-bond chain are considered. In contrast with what occurs for Glauber dynamics, in these two models the dynamic critical exponent turns out to be the same. The alternating isotopic chain with the restricted dynamics is shown to lead to Nagel scaling for temperatures above some critical value. Further support is given relating the Nagel scaling to the existence of multiple (simultaneous) relaxation processes, the dynamics apparently not playing the most important role in determining such scaling.

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I. INTRODUCTION

The scaling hypothesis of Halperin and Hohenberg [1] relates the time scale τ and the correlation length ξ, and introduces the dynamic critical exponent z. In the case of Ising models, z was for a long time believed to be universal, depending on the nature of conserved quantities and of those features, for instance dimensionality [2], which determine their static universality class. However, it is now well established that for some simple systems this exponent is nonuniversal [3–9]. In particular, in the case of one-dimensional Glauber dynamics [10] the alternating isotopic chain [7] presents a universal behavior (in the sense that it leads to the same value of the dynamic critical exponent as the homogeneous chain), whereas the alternating-bond chain does not [7–18] (however, see Ref. [19]). This breakdown of the dynamic scaling hypothesis is due to the different energy barriers determining the diffusion constant and the correlation length, and hence entering into the value of the dynamic exponent z. This exponent is also typically strongly affected when the dynamics takes place on a self-similar background. For instance, the study of the Glauber dynamics in branching and nonbranching Koch curves as well as in the Sierpinsky gasket [20] indicates that z is non universal. Nevertheless, an analysis of the critical Glauber dynamics on the Fibonacci-chain quasicrystal [9] shows that the dynamic exponent z is identical to that obtained for the alternating-bond Glauber chain. Another interesting line of research that was also followed [8] is to understand how different dynamics affect the universality. This work is partly aimed as another contribution to such an understanding.

Kinetic Ising models were also used in a variety of contexts not limited to critical dynamics. In fact, in a previous paper [21] we introduced a quasi-one-dimensional kinetic Ising-like model to study relaxation phenomena in linear polymeric chains, including a region close to the glass transition. In our original model the chains are made up of N segments, each of which may be found in two possible orientations, and the Hamiltonian was chosen so as to reduce to one giving the intramolecular energy of the Gibbs–di Marzio lattice model [22]. For the stochastic dynamics, we adopted a rule of transition for the configurational changes which was tied to the creation or disappearance of flexes. As a consequence of this restricted dynamics, only some states are selected, and, in magnetic language, this implies that in the model the domain wall motion is through a biased random walk. The purpose of this paper is, on the one hand, to introduce restricted dynamics into two one-dimensional alternating kinetic Ising models that have exact solutions with the Glauber dynamics, namely, the isotopic alternating chain and the alternating-bond chain. On the other hand, we will use these extensions to examine the dynamical critical exponent and, in the case of the isotopic chain, whether the inclusion of several relaxation times may be related to multifractal behavior. This last goal is motivated by the fact that recent dielectric susceptibility measurements in several glass-forming systems, and covering wide ranges of temperature and frequency [23–25], suggested that the master curve in which all measurements are shown to scale (the Nagel plot) may be understood in terms of multiple relaxation processes. In fact the existence of simultaneous relaxation processes is assumed to be connected to multifractality, much in the same way that this concept is present in theories of chaos. Very recently we showed that an alternating isotopic chain with Glauber dynamics leads to Nagel scaling [26], and the question arises as to the role that a particular dynamics may play in such a scaling. By examining the model with a restricted dynamics, we aim at shedding some light into this issue.

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The paper is organized as follows. Section II deals with an alternating isotopic chain, while Sec. III is devoted to an alternating-bond chain. We derive the wave-vector frequency-dependent susceptibility, the equations governing the time evolution of the wave-vector-dependent magnetization, and the critical exponent z in both cases. In Sec. IV we address the issue of whether the restricted dynamics leads to a Debye-like scaling of the response functions (as in the uniform chain), or whether the so-called Nagel plot is useful in the case of an isotopic alternating chain. We close the paper in Sec. V with some concluding remarks.

II. ALTERNATING ISOTOPIC CHAIN

The model consists of a closed linear chain with N sites occupied by two isotopes (characterized by two different spin relaxation times) that are alternately arranged. The Hamiltonian is the usual Ising Hamiltonian given by

$$H=-J\sum_{j=1}^{N}\sigma_j\sigma_{j+1}, \tag{1}$$

where σ_j is a stochastic (time-dependent) spin variable assuming the values ± 1, and J is the coupling constant. The configuration of the chain is specified by the set of values $\{\sigma_1,\sigma_2,\ldots,\sigma_N\}$ at time t. As will be argued below, the Hamiltonian will turn out to be not all that relevant in the specific calculations. Nevertheless it is necessary to define the states involved in allowed transitions.

Instead of considering the Glauber dynamics, we assume a kind of transition associated with the motion of domain walls. The idea is similar but not identical to previous work by others in which either the domain wall motion is strongly suppressed at low temperatures [3,4] or is through a one-dimensional random walk [27]. In our case the transition associated with the ith spin takes the form

$$T_i\{\sigma_1,\ldots,\sigma_i,\sigma_{i+1},\ldots,\sigma_{N-1},\sigma_N\}\rightarrow \{\sigma_1,\ldots,\sigma_{i-1},-\sigma_i,\sigma_{i+1},\ldots,\sigma_{N-1},\sigma_N\}, \tag{2}$$

and we impose a biased random walk for the domain wall motion [28]. In order to also account for the presence of the isotopes, we take the transition probabilities to be given by

$$w_i(\sigma_{i-1},\sigma_i)=\alpha_i(1-\gamma\sigma_{i-1}\sigma_i). \tag{3}$$

Here $\gamma=\tanh(J/k_BT)$, k_B being the Boltzmann constant and T the absolute temperature, and α_i is the inverse of the relaxation time τ_i of spin i in the absence of spin interactions. It should be pointed out that the rule of transition stated in Eq. (2) allows for single site excitations such that the transitions are not correlated. Further, the choice made in Eq. (3) immediately implies that detailed balance does not hold for this model and also that not every state in the phase space of the system is accessible. In particular, one should note that within this model no equilibrium state exists, although when the time goes to infinity a steady state is eventually attained. This feature is shared by other purely stochastic models such as the biased Ising lattice gas and its many variations [29].

If we now let α_1 and α_2 represent the inverses of the free spin relaxation times of chains composed solely of spins of species 1 or 2, respectively, then we can set $\alpha_i=\overline{\alpha_1}-(-1)^i\overline{\alpha_2}$, where $\overline{\alpha_1}=(\alpha_1+\alpha_2)/2$ and $\overline{\alpha_2}=(\alpha_1-\alpha_2)/2$.

The time dependent probability $P(\sigma_1,\sigma_2,\ldots,\sigma_N;t)\equiv P(\{\sigma^N\},t)$ for a given spin configuration satisfies the master equation

$$\frac{dP(\{\sigma^N\},t)}{dt}=-\sum_{i=1}^{N}w_i(\sigma_{i-1},\sigma_i)P(\{\sigma^N\},t)+\sum_{i=1}^{N}w_i(\sigma_{i-1},-\sigma_i)P(T_i\{\sigma^N\},t). \tag{4}$$

The dynamical properties we are interested in require a knowledge of some moments of the probability $P(\{\sigma^N\},t)$. Hence we introduce expectation values and correlation functions defined as

$$q_i(t)=\langle\sigma_i(t)\rangle=\sum_{\{\sigma^N\}}\sigma_iP(\{\sigma^N\},t), \tag{5}$$

$$r_{i,j}(t)=\langle\sigma_i(t)\sigma_j(t)\rangle=\sum_{\{\sigma^N\}}\sigma_i\sigma_jP(\{\sigma^N\},t) \tag{6}$$

and

$$c_{i,j}(t',t'+t)=\Theta(t)\langle\sigma_i(t')\sigma_j(t'+t)\rangle=\sum_{\{\sigma^N\},\{\sigma^{N'}\}}\sigma_i'P(\{\sigma^{N'}\},t')\sigma_jp(\{\sigma^N\}|\{\sigma^{N'}\},t), \tag{7}$$

where $\Theta(t)$ is the Heaviside step function, and the sums run over all possible configurations compatible with our rule of motion. The second equality of Eq. (7), which gives a formal definition of the time-delayed correlation function, involves $p(\{\sigma^N\}|\{\sigma^{N'}\},t)$, the conditional probability of the chain having the configuration $\{\sigma^N\}$ at time $t'+t$ provided it had the configuration $\{\sigma^{N'}\}=\{\sigma_1',\sigma_2',\ldots,\sigma_N'\}$ at time t'. Multiplying the master equation by the appropriate quantities, and performing the required summations, we obtain the set of time evolution equations that will be used in our later development. These are given by

$$\frac{dq_j}{dt}=-2\alpha_j(q_j-\gamma q_{j-1}) \tag{8}$$

and

$$\frac{dc_{i,j}(t',t'+t)}{dt}=r_{i,j}(t')\delta(t)-2\alpha_j[c_{i,j}(t',t'+t)-\gamma c_{i,j-1}(t',t'+t)]. \tag{9}$$

We now impose translational invariance, and introduce $\tilde{q}_k$, the (spatial) Fourier transform of q_j, the $t' \to \infty$ limit of the (temporal) Fourier transform of $c_l(t',t'+t) \equiv c_{i,j}(t',t'+t)$ (with $l=j-i$) denoted by $\hat{c}_l(\omega)$, and $\tilde{C}_k(\omega)$, the spatial Fourier transform of $\hat{c}_l(\omega)$, defined through

$$q_j = \frac{1}{\sqrt{N}} \sum_k \tilde{q}_k \exp(ikj), \tag{10}$$

$$\hat{c}_l(\omega) = \lim_{t' \to \infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} c_l(t',t'+t) \exp(-i\omega t) dt, \tag{11}$$

and

$$\tilde{C}_k(\omega) \equiv \langle \sigma_{-k} \sigma_k \rangle_\omega = \frac{1}{N} \sum_l \hat{c}_l(\omega) \exp(-ikl). \tag{12}$$

In terms of these quantities, Eqs. (8) and (9) may be rewritten, as

$$\frac{d\Psi_k}{dt} = \mathbf{M}_k \Psi_k \tag{13}$$

and

$$i\omega \hat{c}_l(\omega) = r_l^\infty - 2\alpha_l [\hat{c}_l(\omega) - \gamma \hat{c}_{l-1}(\omega)], \tag{14}$$

respectively, where

$$\Psi_k = \begin{pmatrix} \tilde{q}_k \\ \tilde{q}_{k-\pi} \end{pmatrix}, \tag{15}$$

$$\mathbf{M}_k = \begin{pmatrix} -2\overline{\alpha}_1 (1-\gamma e^{-ik}) & 2\overline{\alpha}_2 (1+\gamma e^{-ik}) \\ 2\overline{\alpha}_2 (1-\gamma e^{-ik}) & -2\overline{\alpha}_1 (1+\gamma e^{-ik}) \end{pmatrix}. \tag{16}$$

$r_l^\infty = \lim_{t \to \infty} r_l(t)$ is the value of the pair correlation function corresponding to the stationary solution of the equations of motion in the limit $t \to \infty$.

The solution to Eq. (13), which yields the magnetization, is straightforward, namely,

$$\Psi_k(t) = e^{\mathbf{M}_k t} \Psi_k(0). \tag{17}$$

The relaxation process of the wave-vector dependent magnetization is determined by the eigenvalues of $\mathbf{M}_k$. These are given by

$$\lambda_k^\pm = -2\overline{\alpha}_1 \pm 2\sqrt{\overline{\alpha}_1^2 - (\overline{\alpha}_1^2 - \overline{\alpha}_2^2)(1-\gamma^2 e^{-2ik})}. \tag{18}$$

It should be stressed that the eigenvalues $\lambda_k^\pm$ contain both real and imaginary components. Therefore, the relaxation related to the real part of the eigenvalues will in general be modulated by the imaginary component, and care should be taken in defining an adequate correlation length for the critical dynamics. In fact, one can also associate this correlation length with the modulation of the oscillations. Such a correlation length diverges at the critical point, and hence the modulation eventually dissapears. This kind of behavior was already thoroughly discussed in the context of the one-dimensional isotropic ferromagnetic XY model in an inhomogeneous transverse field [30]. In any case, the inverses of the (k-dependent) relaxation times $\tau_k^\pm$ of the $\pm k^{th}$ modes are obtained from the real part of $\lambda_k^\pm$. In the critical region, that is when $T \to 0$ and $k \to 0$, $\lambda_k^- \to -4\overline{\alpha}_1$, while $\lambda_k^+ \to 0$. This means that the critical mode is the one corresponding to λ_k^+. As for the relaxation time, in this limit one obtains

$$\mathrm{Re}(-\lambda_k^+) = -\frac{1}{\tau_k} \sim \frac{4(\overline{\alpha}_1^2 - \overline{\alpha}_2^2)}{\overline{\alpha}_1} \xi^{-2} \left[1 + \frac{(\xi k)^2}{2} \right], \tag{19}$$

where we have identified the correlation length ξ as $\xi \sim e^{J/k_B T}$ by comparing the former expression with the one of the dynamic scaling hypothesis $1/\tau_k \sim \xi^{-z} f(\xi k)$. Therefore we find $z=2$, which is precisely the same result as for the alternating isotopic Glauber chain [7]. Note, however, that this correlation length corresponds to the one of an Ising model with an effective exchange constant $J/2$. This can be easily seen by noting that the equations of motion for the two-spin correlations are in our case formally identical to those in the Glauber chain, but in the latter $\gamma_G = \tanh(2J/k_B T)$. Interestingly enough, ξ also corresponds, as expected, to the correlation length of the steady state attained by the system. The role of the effective constant $J/2$ was already pointed out in the case of the model introduced in Ref. [21].

Now we turn to the calculation of the other interesting response function, namely, the frequency and wave-vector-dependent susceptibility $S_k(\omega)$, which, by virtue of the fluctuation-dissipation theorem [31], is defined by

$$S_k(\omega) = \frac{\langle \sigma_k \sigma_{-k} \rangle_\infty}{k_B T} - \frac{i\omega \langle \sigma_k \sigma_{-k} \rangle_\omega}{k_B T}, \tag{20}$$

where $\langle \sigma_k \sigma_{-k} \rangle_\infty = 1/(1-\gamma \cos k) \cosh(J/k_B T)$ is the static correlation function, and $\langle \sigma_k \sigma_{-k} \rangle_\omega$ the Fourier transform of the dynamic one. After some rather lengthy but not too complicated algebraic manipulations starting with Eq. (14), we arrive at

$$S_k(\omega) = \frac{1}{k_B T (1-\gamma \cos k) \cosh \dfrac{J}{k_B T}} \times \left[1 - \frac{i\omega [i\omega + 2\overline{\alpha}_1 (1+\gamma e^{-ik})]}{(i\omega + 2\overline{\alpha}_1)^2 - 4\overline{\alpha}_2^2 + 4\gamma^2 (\overline{\alpha}_2^2 - \overline{\alpha}_1^2) e^{-2ik}} \right]. \tag{21}$$

The result embodied in Eq. (21) constitutes the proper framework in which to discuss the issue of Nagel scaling in the relaxation of a linear chain with translational invariance and restricted dynamics. This will be postponed until Sec. IV. For the time being, we just quote the equivalent result for the isotopic chain with Glauber dynamics [7,26], namely,

$$S_k^G(\omega)=\frac{1}{k_BT(1-\gamma_G\cos k)\cosh\dfrac{2J}{k_BT}}\times\left[1-\frac{i\omega[i\omega+\overline{\alpha}_1(1+\gamma_G\cos k)]}{(i\omega+\overline{\alpha}_1)^2-\dfrac{1}{2}\gamma_G^2\alpha_1\alpha_2(1+\cos 2k)-\overline{\alpha}_2^2}\right], \tag{22}$$

which is also required for such a discussion. In the next Sec. III we will consider the other simple alternating Ising chain including the dynamics allowed by our rule of transition.

III. ALTERNATING-BOND CHAIN

The model consists of a closed linear chain with N sites, and is characterized by different coupling constants J_j (to be specified below). N is taken to be an even integer, and periodic conditions are also imposed. This model can be applied in the description of dimerized structures and the Hamiltonian is again of the Ising type, i.e.,

$$H=-\sum_{j=1}^{N} J_j\sigma_j\sigma_{j+1}, \tag{23}$$

where the parameters and variables are defined as in Sec. II Once more, and for the same reasons as above, we specify the Hamiltonian to have a precise definition of the states that intervene in allowed transitions, but it will play no further relevant role in the calculations that follow.

Considering again the same kind of biased random walk for the domain wall motion and the rule of transition given by Eq. (2), in this case the transition probabilities are taken to be

$$w_i(\sigma_{i-1},\sigma_i)=\alpha(1-\beta_{i-1}\sigma_{i-1}\sigma_i), \tag{24}$$

where α is the inverse of the free spin relaxation time, $\beta_j=\tanh(J_j/k_BT)$, and $J_j=\frac{1}{2}(J_1+J_2)-[(-1)^j/2](J_1-J_2)$. Here J_1 and J_2 represent the coupling constants of two different uniform Ising chains, respectively. It is also convenient to introduce the quantities $\gamma_1=\frac{1}{2}[\tanh(J_1/k_BT)+\tanh(J_2/k_BT)]$ and $\gamma_2=\frac{1}{2}[\tanh(J_1/k_BT)-\tanh(J_2/k_BT)]$, so that β_j may be expressed as $\beta_j=\gamma_1-(-1)^j\gamma_2$. The analogous forms of Eqs. (8) and (9), obtained using a similar procedure, read

$$\frac{dq_j}{dt}=-2\alpha(q_j-\beta_{j-1}q_{j-1}) \tag{25}$$

and

$$\frac{dc_{i,j}(t',t'+t)}{dt}=r_{i,j}(t')\delta(t)-2\alpha[c_{i,j}(t',t'+t)-\beta_{j-1}c_{i,j-1}(t',t'+t)]. \tag{26}$$

As in the previous case, we now impose translational invariance, and again use $\tilde{q}_k$, $\hat{c}_l(\omega)$, and $\tilde{C}_k(\omega)$, defined in Sec. II to rewrite Eqs. (25) and (26) as

$$\frac{d\Phi_k}{dt}=\mathbf{N}_k\Phi_k \tag{27}$$

and

$$i\omega\hat{c}_l(\omega)=r_l^{\infty}-2\alpha[\hat{c}_l(\omega)-\beta_{l-1}\hat{c}_{l-1}(\omega)], \tag{28}$$

where

$$\Phi_k=\begin{pmatrix}\tilde{q}_k\\ \tilde{q}_{k-\pi}\end{pmatrix}, \tag{29}$$

$$\mathbf{N}_k=\begin{pmatrix}-2\alpha(1-\gamma_1e^{-ik}) & -2\alpha\gamma_2e^{-ik}\\ 2\alpha\gamma_2e^{-ik} & -2\alpha(1+\gamma_1e^{-ik})\end{pmatrix}. \tag{30}$$

The solution to Eq. (27), which yields the magnetization, is again straightforward, namely,

$$\Phi_k(t)=e^{\mathbf{N}_kt}\Phi_k(0). \tag{31}$$

The eigenvalues of $\mathbf{N}_k$ may be obtained very easily with the result

$$\overline{\lambda}_k^{\pm}=-2\alpha(1\pm\sqrt{\gamma_1^2e^{-2ik}-\gamma_2^2e^{-2ik}}), \tag{32}$$

and again contain real and imaginary components. Proceeding as in the derivation of Eq. (19), we find that the critical mode corresponds to $\overline{\lambda}_k^-$, and that the relaxation time is given by

$$\mathrm{Re}(-\overline{\lambda}_k^-)=\frac{1}{\overline{\tau}_k}\sim 2\alpha\overline{\xi}^{-2}\left[1+\frac{(\overline{\xi}k)^2}{2}\right]. \tag{33}$$

Here, considering that $J_1>J_2$, the correlation length $\overline{\xi}$ has been identified as $\overline{\xi}\sim e^{J_2/k_BT}$ by again comparing Eq. (33) with the dynamic scaling hypothesis $1/\overline{\tau}_k\sim\overline{\xi}^{-z}f(\overline{\xi}k)$. Therefore, we also find $z=2$ in this case, which coincides with the result derived above for the isotopic chain and, consequently, the restricted dynamics produces a dynamic critical exponent which is independent of the kind of interactions in these models. Note that once more the correlation length $\overline{\xi}$ corresponds to that of an Ising model with an effective constant $J_2/2$.

The dynamic scaling exponent z may also be derived in this case by an alternative argument based on domain wall motion. Consider the limit $T\to 0$, in which critical slowing down occurs and domains are formed. According to Eq. (24), if a spin j is in the interior of the domain, in this limit $w_j(\sigma_{j-1},\sigma_j)\to 0$ irrespective of the value of β_{j-1}; on the other hand, if spin i belongs to a domain wall, $w_i(\sigma_{i-1},\sigma_i)\to 2\alpha$, also independently of β_{i-1}. Therefore,

in the low temperature limit, $w_j \ll w_i$, so that the dynamics of the system is equivalent to a biased random motion of the domain wall for the Hamiltonian system, in this instance the Ising model. Hence, within restricted dynamics, the relaxation time $\overline{\tau_0}$ for the decay of a domain of size $\overline{\xi}$ (which is the correlation length associated with the steady state of the stochastic model) is such that $\overline{\tau_0} \sim \overline{\xi}^z$, and may be related to a biased random walk [5]. To this end, let N_0 be the number of spins that must flip to obtain a domain of size ξ_I (the correlation length of the Ising model). Since the domain has the size of the biased random walk with N_0 steps and $z=1$ for the biased random walk, $\xi_I \sim N_0$. On the other hand, $\overline{\tau_0} \sim N_0 w_i^{-1} \sim \xi_I/(2\alpha)$. But $\xi_I = \overline{\xi}^2$, so that $z=2$ for the alternating-bond model for any choice of J_1 and J_2.

Finally, for the sake of completeness, we will also compute the frequency and wave-vector-dependent susceptibility $\overline{\chi_k}(\omega)$ of this model. Taking the same steps as in the case of the isotopic chain, we find

$$\overline{S_k}(\omega) = \frac{\langle \sigma_k \sigma_{-k} \rangle_\infty}{k_B T} \left[1 - \frac{i\omega(i\omega + 2\alpha + 2\alpha\gamma_1 e^{-ik})}{(i\omega + 2\alpha)^2 + 4\alpha^2 e^{-2ik}(\gamma_2^2 - \gamma_1^2)} \right] + \frac{\langle \sigma_k \sigma_{-k+\pi} \rangle_\infty}{k_B T} \frac{2i\omega\alpha\gamma_2 e^{-ik}}{(i\omega + 2\alpha)^2 + 4\alpha^2 e^{-2ik}(\gamma_2^2 - \gamma_1^2)}, \tag{34}$$

with

$$\langle \sigma_k \sigma_{-k} \rangle_\infty = \frac{(1-u_1u_2)[1 + u_1u_2 + (u_1+u_2)\cos k]}{1 + u_1^2 u_2^2 - 2u_1u_2 \cos 2k}, \tag{35}$$

$$\langle \sigma_k \sigma_{-k+\pi} \rangle_\infty = \frac{i(1+u_1u_2)(u_2-u_1)\sin k}{1 + u_1^2 u_2^2 - 2u_1u_2 \cos 2k}, \tag{36}$$

and $u_j = \tanh(J_j/2k_BT)$, $j=1$ and 2. Again for the sake of comparison, and in order to correct a misprint in the formula that appeared in Ref. [7], we quote the equivalent results using the Glauber dynamics, namely,

$$\overline{S_k^G}(\omega) = \frac{\langle \sigma_k \sigma_{-k} \rangle_\infty^G}{k_B T} \left[1 - \frac{i\omega(i\omega + \alpha + 2\alpha\gamma'^G \cos k)}{(i\omega+\alpha)^2 - 2\alpha^2[(\gamma'^G)^2 - (\delta^G)^2]\cos 2k - 2\alpha^2[(\gamma'^G)^2 + (\delta^G)^2]} \right] + \frac{\langle \sigma_k \sigma_{-k+\pi} \rangle_\infty^G}{k_B T} \frac{2\alpha\delta^G \omega \sin k}{(i\omega+\alpha)^2 - 2\alpha^2[(\gamma'^G)^2 - (\delta^G)^2]\cos 2k - 2\alpha^2[(\gamma'^G)^2 + (\delta^G)^2]}, \tag{37}$$

with

$$\langle \sigma_k \sigma_{-k} \rangle_\infty^G = \frac{(1-u_1^G u_2^G)[1 + u_1^G u_2^G + (u_1^G + u_2^G)\cos k]}{1 + (u_1^G u_2^G)^2 - 2u_1^G u_2^G \cos 2k}, \tag{38}$$

$$\langle \sigma_k \sigma_{-k+\pi} \rangle_\infty^G = \frac{i(1+u_1^G u_2^G)(u_2^G - u_1^G)\sin k}{1 + (u_1^G u_2^G)^2 - 2u_1^G u_2^G \cos 2k}, \tag{39}$$

$\gamma'^G = \frac{1}{2}\tanh[(J_1+J_2)/k_BT]$, $\delta^G = -\frac{1}{2}\tanh[(J_1-J_2)/k_BT]$, and $u_j^G = \tanh(J_j/k_BT)$, and $j=1$ and 2. This concludes our analysis of the alternating-bond chain with the restricted dynamics.

IV. SUSCEPTIBILITY AND SCALING BEHAVIOR

Thus far, we have examined the behavior of the critical dynamic exponent. In this section we will continue our exploration by considering the scaling properties of the susceptibility in the isotopic alternating chain. This is most conveniently done through the quantity $\chi(\omega) \equiv k_B T S_0(\omega)/\langle \sigma_0 \sigma_0 \rangle_\infty$. It should be noted that if we look at the uniform chain, i.e., set $\alpha_1 = \alpha_2$ in Eq. (21) and take the limit $k=0$ in the resulting expression, χ obeys the usual normalized Debye scaling: if one scales the frequency with the inverse of the (single) relaxation time, and the real and imaginary parts are then divided by their values at 0 and 1, respectively, one obtains a universal curve. However, as mentioned in Sec. I, recently experimental work on dielectric relaxation was reported in terms of a new scaling function [23–25] which is thought to be related to multifractal scaling. In this scaling, the abscissa is $(1+W)\log_{10}(\omega/\omega_p)/W^2$, and the ordinate is $\log_{10}[\chi''(\omega)\omega_p/\omega\Delta\chi]/W$. Here χ'' is the imaginary part of $\chi(\omega)$, W is the full width at half maximum of χ'', ω is the frequency, ω_p corresponds to the peak in χ'', and $\Delta\chi = \chi(0) - \chi_\infty$ is the static susceptibility. It is therefore interesting to see whether the isotopic alternating chain with the restricted dynamics leads to Nagel scaling in the same way that the model with Glauber dynamics does [26].

Using Eqs. (18) and (21) with $k=0$, χ can be expressed in the form

$$\chi(\omega) = \frac{(1-\gamma)(\alpha_1+\alpha_2)}{2} \times \left[\frac{1 - f(\alpha_1,\alpha_2,\gamma)}{i\omega - \lambda_0^+} - \frac{1 + f(\alpha_1,\alpha_2,\gamma)}{i\omega - \lambda_0^-} \right]. \tag{40}$$

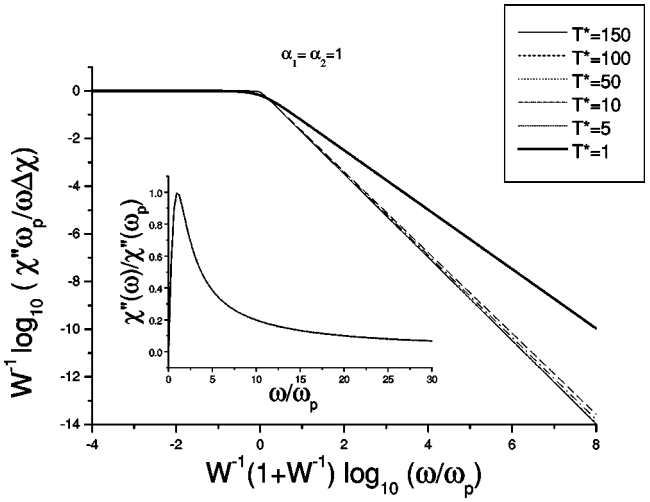

FIG. 1. Nagel plot for the case of a uniform chain ($\alpha_1=\alpha_2=1$). Note that the proposed scaling does not hold in this case, while, as the inset shows, the susceptibility obeys the usual Debye scaling.

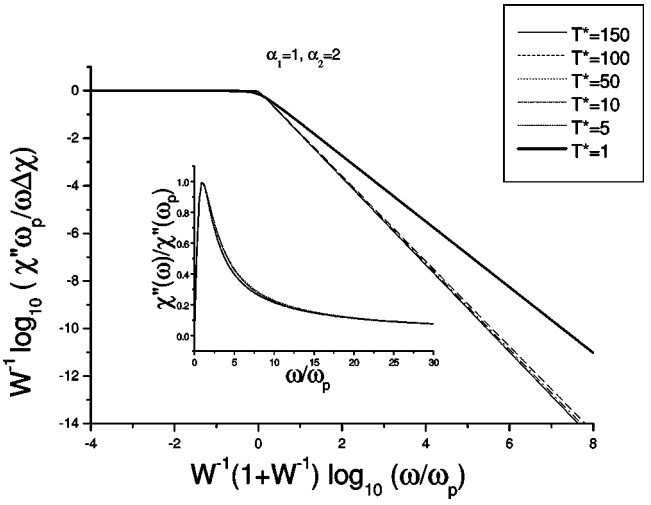

FIG. 2. Nagel plot for $\alpha_1=1$ and $\alpha_2=2$. Here one can see an improvement of the scaling behavior as compared to the uniform chain case, except at low T^*. In the inset the plot to test the performance with respect to the Debye scaling is presented.

Here, the (temperature dependent) function $f(\alpha_1,\alpha_2,\gamma)$ is given by

$$f(\alpha_1,\alpha_2,\gamma)=\frac{(\alpha_1-\alpha_2)^2-4\alpha_1\alpha_2\gamma^2}{(\alpha_1+\alpha_2)\sqrt{(\alpha_1-\alpha_2)^2+4\alpha_1\alpha_2\gamma^2}}. \quad (41)$$

It should be pointed out that for the case $\gamma=0$, we obtain

$$\chi_{\gamma=0}=\frac{\alpha_1}{i\omega+2\alpha_1}+\frac{\alpha_2}{i\omega+2\alpha_2}, \quad (42)$$

so that the general structure of the result for the susceptibility of the alternating isotopic chain is preserved irrespective of the value of γ (i.e., of the temperature), namely a linear combination of two Debye-like terms.

With the aid of Eqs. (40) and (41), in Figs. 1–4 we present Nagel plots for the cases $\alpha_1=\alpha_2=1$, $\alpha_1=1$, and $\alpha_2=2$, $\alpha_1=1$ and $\alpha_2=100$, and $\alpha_1=1$ and $\alpha_2=1000$, respectively, and different values of $1/T^*\equiv J/k_BT$. In these figures we also include plots of $\chi''(\omega)$ vs ω/ω_p which are the natural variables of the Debye relaxation. While the first case (which as stated above corresponds to Debye behavior) does not show Nagel scaling, the situation somewhat improves in the second one (where clearly improvement means less dispersion in the curves), and when the two relaxation times are not only different but very far apart (third and fourth cases) the scaling is virtually perfect, provided the temperature lies above some certain critical value. For comparison, in Fig. 5 we show parallel results computed for the alternating isotopic chain with Glauber dynamics [cf. Eq. (22)], for the case $\alpha_1=1$ and $\alpha_2=100$. The similarity of the results of both models provides support to the idea that, irrespective of the specific dynamics, the coexistence of different relaxation mechanisms lies behind the Nagel scaling, and that this only occurs if a threshhold temperature is surpassed. Nevertheless, the character of the different dynamics manifests itself in the fact that the slopes of the decaying parts of the curves in the Nagel plot differ and the fact that, for the same values of α_1 and α_2, the scaling is more closely followed by the model with the restricted dynamics (cf. Figs. 3 and 5).

It should be noted that, as the insets of these figures indicate, both types of dynamics lead to two peaks in $\chi''(\omega)$ due to the presence of two different relaxation times. This feature was also observed experimentally by Dixon *et al.* [23], Lesley-Pelecky and Birge [24], and Wu *et al.* [25] in different materials, and associated with the α and β relaxations. Very recently it was also confirmed in experiments by Brand *et al.* [32], who also noted the presence of a third relaxation process unexplained so far.

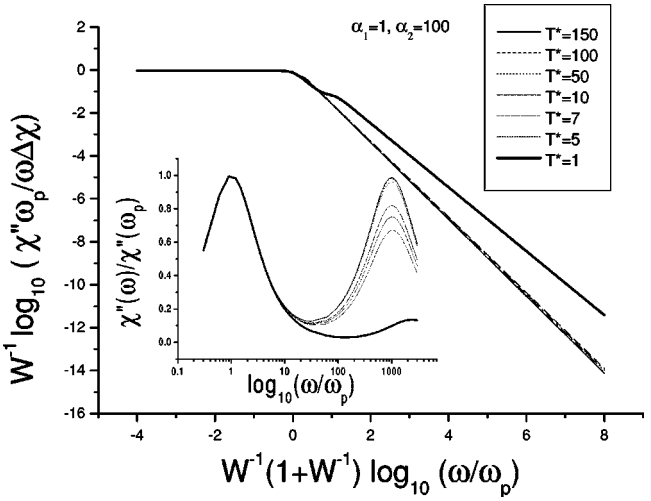

FIG. 3. Same as Fig. 2, but for the choices $\alpha_1=1$ and $\alpha_2=100$. Except at low T^* values, the trend of improvement of the agreement with the Nagel scaling is apparent, while the opposite happens with respect to the Debye scaling.

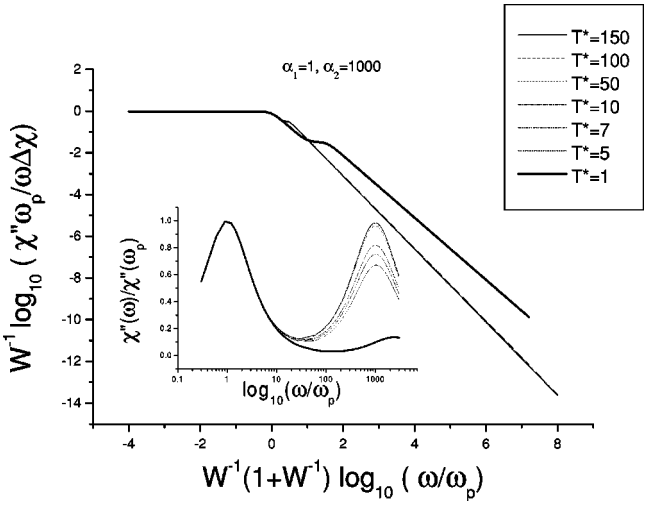

FIG. 4. Same as Figs. 2 and 3, but for $\alpha_1=1$ and $\alpha_2=1000$. The scaling is virtually perfect in this case, except at low T^*. Note the explicit appearance of a plateau region in the plot. The behavior here is definitely non-Debye.

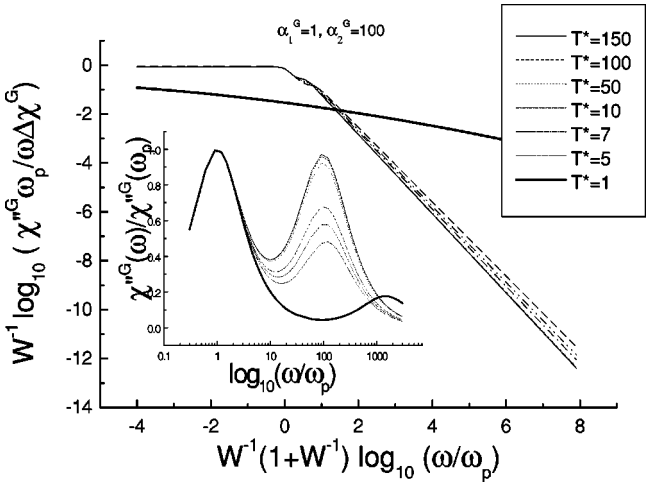

FIG. 5. Nagel plot for an alternating isotopic chain with Glauber dynamics with $\alpha_1=1$ and $\alpha_2=100$ and different values of the parameter $T_G^*\equiv k_BT/2J$. Here $\chi^G(\omega)\equiv k_BTS_0^G(\omega)/\langle\sigma_0\sigma_0\rangle_\infty^G$, with $\langle\sigma_0\sigma_0\rangle_\infty^G=1/(1-\gamma_G)\cosh(1/T_G^*)$ and $S_0^G(\omega)$ computed with the aid of Eq. (22). Note the similarity of these results with respect to those of Fig. 3.

V. CONCLUDING REMARKS

In this paper we addressed relaxation processes and the question of the value of the dynamical critical exponent in kinetic Ising models on alternating linear chains. Two different issues were examined in this context. In the first one, we showed that with the restricted dynamics implied by the transition probabilities [cf. Eqs. (3) and (24)], both in an alternating-bond chain and in an isotopic chain the dynamic critical exponent z turns out to be exactly 2. This does not occur if the Glauber dynamics is employed. Hence the value of the dynamic critical exponent and the dynamics implied by the rule of transition in kinetic models are deeply related. As for the second issue, an analysis of Nagel plots in the case of an alternating isotopic chain indicates that the presence of at least two different relaxation mechanisms is required for the scaling of the susceptibility. This feature agrees with what one finds with the usual Glauber dynamics [26], as well as the appearance of plateau regions in the plot if the relaxation times are widely separated, and of the existence of a critical temperature below which the scaling is not followed. One may reasonably wonder at this stage whether an alternating-bond chain with restricted dynamics also obeys the Nagel scaling. Since for high temperatures this model is equivalent to a chain with a single relaxation time, it is not surprising that the scaling is not followed in this instance. We have confirmed this numerically for a variety of values for J_1 and J_2.

Although our results for the isotopic chain suggest that the dynamics seems not to play a key role for the scaling to hold, one should bear in mind that an isotopic chain with restricted dynamics containing only two isotopes is somewhat peculiar, so that no definite conclusions on this issue can be reached at this stage. Concerning the differences, it is conceivable that stochasticity may well be behind the fact that the slope of the decaying parts of the curves in the Nagel plots is larger for the restricted dynamics than for the Glauber dynamics. In this respect, it is important to point out that experiments in which the Nagel plots have been more succesful concern glass-forming systems and that our original model was built so as to reflect the topological constraints that are assumed to be crucial in such systems. It is clear that the restricted dynamics related to such constraints is also not enough to obtain the scaling, as exemplified by the case of the uniform chain $\alpha_1=\alpha_2=1$. The true alternating isotopic chain with restricted dynamics examined here, on the other hand, includes both ingredients, and provides a *bona fide microscopic model* in which the Nagel scaling is shown to arise. Moreover, the fact that we obtain a larger slope in the restricted model is consistent with the experimental finding that such a slope is larger for the orientationally disordered crystalline phase of cyclo-octanol (cf. Lesley-Pelecky and Birge [24]) than in the originally studied linear polymers [25].

Notwithstanding the limitations of this model, our expectation is that both our earlier results [21,26] and the present ones provide some insight into the physical origin and validity of the hypothesis concerning the need for the simultaneous presence of multiple relaxation mechanisms as related to the proposal of the Nagel plots. A future challenge is to examine whether Nagel scaling is also present in other Ising models recently studied in connection with glassy dynamics [33], which are based on the spin facilitated models originally introduced by Fredrickson and Andersen [34]. Finally, one can conjecture that the appearance of a third relaxation process, as observed in the recent experiments of dielectric relaxation by Brand *et al.* [32], may be hopefully catered for within our model through the inclusion of a third relaxation time. The investigation of this conjecture is presently in progress.

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[1] B.I. Halperin and P.C. Hohenberg, Phys. Rev. **177**, 952 (1969); P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[2] An odd case in this respect is the Gaussian model. Very recently, it was shown that in this model z has the same value independent of spatial dimensionality [J.-Y. Zhu and Z.R. Yang, Phys. Rev. E **59**, 1551 (1999)].

[3] J.C. Kimball, J. Stat. Phys. **21**, 289 (1979).

[4] U. Deker and F. Haake, Z. Phys. B: Condens. Matter **35**, 281 (1979); F. Haake and K. Thol, *ibid.* **40**, 219 (1980).

[5] R. Cordery, S. Sarker, and J. Tobochnik, Phys. Rev. B **24**, 5402 (1981).

[6] N. Menhyárd and G. Ódor, J. Phys. A **28**, 4505 (1995).

[7] L.L. Gonçalves and N.T. de Oliveira, Can. J. Phys. **63**, 1215 (1985).

[8] M. Droz, J. Kamphorst Leal da Silva, and A. Malaspinas, Phys. Lett. A **115**, 448 (1986); M. Droz, J. Kamphorst Leal da Silva, A. Malaspinas, and A.L. Stella, J. Phys. A **20**, L387 (1987).

[9] J.A. Ashraff and R.B. Stinchcombe, Phys. Rev. B **40**, 2278 (1989).

[10] R.J. Glauber, J. Math. Phys. **4**, 294 (1963).

[11] E.J.S. Lage, J. Phys. C **20**, 3969 (1987).

[12] J.H. Luscombe, Phys. Rev. B **36**, 501 (1987).

[13] J.C. Angles d'Auriac and R. Rammal, J. Phys. A **20**, 763 (1988).

[14] J.M. Nunes da Silva and E.J.S. Lage, J. Stat. Phys. **58**, 115 (1990).

[15] S. Cornell, M. Droz, and N. Menyhárd, J. Phys. A **24**, L201 (1991).

[16] S.J. Cornell, K. Kaski, and R.B. Stinchcombe, J. Phys. A **24**, L865 (1991).

[17] J. Kamphorst Leal da Silva, A.G. Moreira, M. Silvério Soares, and F.C. Sá Barreto, Phys. Rev. E **52**, 4527 (1995).

[18] P. Tong, Phys. Rev. E **56**, 1371 (1997).

[19] B.W. Southern and Y. Achiam, J. Phys. A **26**, 2505 (1993); **26**, 2519 (1993).

[20] Y. Achiam, Phys. Rev. B **31**, 4732 (1985).

[21] M. López de Haro, J. Tagüeña-Martínez, B. Espinosa, and L.L. Gonçalves, J. Phys. A **26**, 6697 (1993); **29**(E), 7353 (1996); M. López de Haro, L.L. Gonçalves, and J. Tagüeña-Martínez, Mod. Phys. Lett. B **10**, 1441 (1996).

[22] J.H. Gibbs and E.A. di Marzio, J. Chem. Phys. **28**, 373 (1958).

[23] P.K. Dixon, L. Wu, S.R. Nagel, B.D. Williams, and J.P. Carini, Phys. Rev. Lett. **65**, 1108 (1990); M.D. Ediger, C.A. Angell, and S.R. Nagel, J. Phys. Chem. **100**, 13 200 (1996).

[24] D.L. Lesley-Pelecky and N.O. Birge, Phys. Rev. Lett. **72**, 1232 (1992).

[25] L. Wu, P.K. Dixon, S. Nagel, B.D. Williams, and J.P. Carini, J. Non-Cryst. Solids **131-133**, 32 (1991).

[26] L.L. Gonçalves, M. López de Haro, J. Tagüeña-Martínez, and R.B. Stinchcombe, Phys. Rev. Lett. **84**, 1507 (2000).

[27] J.L. Skinner, J. Chem. Phys. **79**, 1955 (1983).

[28] See, for instance, B.H. Kaye, *A Random Walk Through Fractal Dimensions*, 2nd ed. (VCH, Weinheim, 1994).

[29] B. Schmittman and R.K.P. Zia, in *Statistical Mechanics of Driven Diffusive Systems, Phase Transitions and Critical Phenomena*, Vol. 17, edited by C. Domb and J.L. Lebowitz (Academic Press, New York, 1995).

[30] J.P. de Lima and L.L. Gonçalves, Mod. Phys. Lett. B **14&15**, 871 (1994).

[31] M. Suzuki and R. Kubo, J. Phys. Soc. Jpn. **24**, 51 (1968).

[32] R. Brand, P. Lunkenheimer, U. Schneider, and A. Loidl, e-print cond-mat/0002460.

[33] E. Follana and F. Ritort, Phys. Rev. B **54**, 930 (1996); M. Schulz and S. Trimper, J. Stat. Phys. **58**, 173 (1999); B. Zheng, M. Schulz, and S. Trimper, Phys. Rev. B **54**, 6717 (1999).

[34] G.H. Fredrickson and H.C. Andersen, Phys. Rev. Lett. **53**, 1244 (1984); J. Chem. Phys. **84**, 5822 (1985).