Nagel Scaling and Relaxation in the Kinetic Ising Model on an n-Isotopic Chain

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The kinetic Ising model on an n-isotopic chain is considered in the framework of Glauber dynamics. The chain is composed of N segments with n sites, each one occupied by a different isotope. Due to the isotopic mass difference, the n spins in each segment have different relaxation times in the absence of interactions, and consequently the dynamics of the system is governed by multiple relaxation mechanisms. The solution is obtained in closed form for arbitrary n, by reducing the problem to a set of n coupled equations, and it is shown rigorously that the critical exponent z is equal to 2. Explicit results are obtained numerically for any temperature and it is also shown that the dynamic susceptibility satisfies the new scaling (Nagel scaling) proposed for glass-forming liquids. This is in agreement with our recent results (L. L. Gonçalves, M. López de Haro, J. Tagüeña-Martínez and R. B. Stinchcombe, *Phys. Rev. Lett.* **84**, 1507 (2000)), which relate this new scaling function to multiple relaxation processes.

Universal behavior in various physical model systems has been one of the clues to uncovering fundamental regularities of nature. About ten years ago, a scaling hypothesis (Nagel scaling) was proposed to describe experimental work on dielectric relaxation in glass-forming liquids[1]. This hypothesis was meant to replace the more usual normalized Debye scaling, where the frequency is scaled with the inverse of the (single) relaxation time and the real and imaginary parts of the dynamic susceptibility are then divided by their values at zero and one, respectively. However, and in spite of its phenomenological success and apparent ubiquity, its physical origin is as yet not quite well understood.

Very recently, we put forward what we believe to be the first *bona fide* microscopic model in which Nagel scaling is shown to arise[2]. In this previous work, we computed the magnetization, the dynamic critical exponent z and the frequency and wavevector dependent susceptibility of the kinetic Ising model on an alternating isotopic chain with Glauber dynamics[3]. Our results indicated that as soon as the two relaxation times of this model became substantially different, the agreement with the Nagel scaling improved significantly. The question remained of whether the inclusion of more relaxation mechanisms would lead to the same sort of results. It is this issue that we mainly want to examine in this paper. Hence we present an extension of the alternating isotopic chain in which rather than only two relaxation times, n relaxation times are involved.

The model consists of a linear chain with N seg-

ments, each one containing n sites occupied by iso-
topes characterized by n different spin relaxation times.
The Hamiltonian for the lth segment is the usual Ising
Hamiltonian given by

$$H_l = -J \sum_{j=1}^{n} \sigma_{l,j} \sigma_{l,j+1}, \qquad (1)$$

where $\sigma_{l,j}$ is a stochastic (time-dependent) spin vari-
able assuming the values ± 1 and J the coupling con-
stant. Note that if $n = 2$, this model reduces to the
alternating isotopic chain treated in Ref. [2]. The con-
figuration of the segment is specified by the set of values
$\{\sigma_{l,1}, \sigma_{l,2}, ...\sigma_{l,n}\} \equiv \{\sigma^{l,n}\}$ at time t. This configura-

tion evolves in time due to interactions with a heat
bath. We assume for the segments the usual Glauber
dynamics so that the transition probabilities are given
by

$$w_{li}(\sigma_{l,i}) = \frac{1}{2}\alpha_i \left(1 - \frac{\gamma}{2}(\sigma_{l,i-1}\sigma_{l,i} + \sigma_{l,i}\sigma_{l,i+1})\right), \quad (2)$$

where $\gamma = \tanh(2J/k_B T)$, 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.

The time dependent probability $P\left(\{\sigma^{l,n}\}, t\right)$ for a
given spin configuration satisfies the master equation

$$
\begin{aligned}
\frac{dP\left(\{\sigma^{l,n}\}, t\right)}{dt} \;=\; & -\sum_{i=1}^{n} w_{li}(\sigma_{l,i}) P\left(\{\sigma^{l,n}\}, t\right) \\
& +\sum_{i=1}^{n} w_{li}(-\sigma_{l,i}) P\left(T_{li}\{\sigma^{l,n}\}, t\right),
\end{aligned}
\qquad (3)
$$

where $T_{li}\{\sigma^{l,n}\} \equiv \{\sigma_{l,1}, \sigma_{l,2}, ...\sigma_{l,i-1}, -\sigma_{l,i}, \sigma_{l,i+1}, ...\sigma_{l,n}\}$. The dynamical properties we are interested in, namely
the magnetization, the dynamic critical exponent and the susceptibility, require the knowledge of some moments of
the probability $P\left(\{\sigma^{l,n}\}, t\right)$. Hence, we introduce the following expectation values defined as:

$$q_{li}(t) = \langle \sigma_{li}(t) \rangle = \sum_{\{\sigma^{l,n}\}} \sigma_{l,i} P\left(\{\sigma^{l,n}\}, t\right), \qquad (4)$$

where the sum runs over all possible configurations. Using the master equation (3) and this definition of $q_{li}(t)$, one
can easily derive the result

$$
\begin{aligned}
\frac{dq_{l,1}}{dt} \;&=\; -\alpha_1 \left(q_{l,1} - \frac{\gamma}{2}(q_{l-1,n} + q_{l,2})\right), \\
\frac{dq_{l,j}}{dt} \;&=\; -\alpha_j \left(q_{l,j} - \frac{\gamma}{2}(q_{l,j-1} + q_{l,j+1})\right), (2 \leq j \leq n-1) \\
\frac{dq_{l,n}}{dt} \;&=\; -\alpha_n \left(q_{l,n} - \frac{\gamma}{2}(q_{l,n-1} + q_{l+1,1})\right).
\end{aligned}
\qquad (5)
$$

Introducing now the Fourier transform $\widetilde{q}_{Q,l}$ ($l = 1, 2, ...n$) defined by

$$\widetilde{q}_{Q,l} = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} \exp(iQld)q_{l,j} \qquad (6)$$

where $Q = \frac{2\pi m}{Nd}$ ($m = 0, 1, 2...N$), $d = na$, a being a lattice parameter and the vector Ψ_Q given by

$$
\Psi_Q = \begin{pmatrix} \widetilde{q}_{Q,1} \\ . \\ . \\ . \\ \widetilde{q}_{Q,n} \end{pmatrix},
\qquad (7)
$$

one can derive the following result

$$\frac{d\Psi_Q}{dt} = \mathbf{M}_Q \Psi_Q \qquad (8)$$

where the matrix $\mathbf{M}_Q$ has a rather suggestive structure given by

$$
\mathbf{M}_Q = \begin{pmatrix}
-\alpha_1 & \frac{\alpha_1 \gamma}{2} & 0 & . & . & 0 & \frac{\alpha_1 \gamma}{2} e^{iQd} \\
\frac{\alpha_2 \gamma}{2} & -\alpha_2 & \frac{\alpha_2 \gamma}{2} & 0 & . & . & 0 \\
0 & \frac{\alpha_3 \gamma}{2} & -\alpha_3 & \frac{\alpha_3 \gamma}{2} & 0 & . & 0 \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & . \\
. & . & . & 0 & \frac{\alpha_{n-1} \gamma}{2} & -\alpha_{n-1} & \frac{\alpha_{n-1} \gamma}{2} \\
\frac{\alpha_n \gamma}{2} e^{-iQd} & 0 & . & . & . & \frac{\alpha_n \gamma}{2} & -\alpha_n
\end{pmatrix}. \tag{9}
$$

The solution to Eq. (8), which yields the magnetization, is straightforward, namely

$$
\Psi_Q(t) = e^{\mathbf{M}_Q t} \Psi_Q(0). \tag{10}
$$

The relaxation process of the wave-vector dependent magnetization is determined by the eigenvalues of $\mathbf{M}_Q$ denoted as λ_{lQ} ($l = 1, 2, ...n$) and which for $n \geq 5$ have to be computed numerically. The same applies to the dynamic critical exponent z, which is obtained by imposing the scaling relation $\tau_Q \sim \xi^z f(\xi Q)$ for the critical mode, λ_{1Q}, with the (Q-dependent) relaxation time $\tau_Q = -\frac{1}{\lambda_{1Q}}$, in the region $T \to 0$ and $Q \to 0$ where $\lambda_{1Q} \to 0$, and the correlation length ξ is $\xi \sim \exp(2J/k_B T)$. This yields

$$
\ln\left(-\frac{1}{\lambda_{1Q}}\right) = C + \frac{2Jz}{k_B T}, \tag{11}
$$

where C is an irrelevant constant. By plotting $\ln\left(-\frac{1}{\lambda_{10}}\right)$ vs. $\frac{2J}{k_B T}$ and considering the limit $T \to 0$, we have checked analytically for $n = 2$[2] and numerically for $n = 3, 4$ and 5 and various values of the $\alpha's$ that $z = 2$, so that this model belongs to the same universality class as the uniform Ising chain.

Let us now introduce the spatial Fourier transform $\hat{c}_Q(t', t' + t)$ of the time-dependent correlation defined by

$$
\hat{c}_Q(t', t' + t) = \frac{1}{nN} \sum_{l=1}^{N} \sum_{l'=1}^{N} \sum_{i=1}^{n} \sum_{j=1}^{n} e^{-iQdl} e^{iQdl'} \langle \sigma_{l,i}(t') \sigma_{l',j}(t' + t) \rangle. \tag{12}
$$

Then, the $t' \to \infty$ limit of the temporal Fourier transform of $\hat{c}_Q(t', t' + t)$, denoted by $\widetilde{C}_Q(\omega)$, is given by

$$
\widetilde{C}_Q(\omega) = \lim_{t' \to \infty} \frac{1}{2\pi n} \sum_{i=1}^{n} \sum_{j=1}^{n} \int_{-\infty}^{\infty} \langle \widetilde{\sigma}_{-Q,i}(t') \widetilde{\sigma}_{Q,j}(t' + t) \rangle \exp(-i\omega t) dt, \tag{13}
$$

with $\widetilde{\sigma}_{Q,m} = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} \exp(iQld)\sigma_{l,m}$. After some lengthy and tedious but not very difficult algebra, using eq. (4) and the above definitions one may derive the result

$$
\widetilde{C}_Q(\omega) = \sum_{l=1}^{n} \frac{g_{lQ}}{i\omega - \lambda_{lQ}} \tag{14}
$$

where

$$
g_{lQ} = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{m=1}^{n} \frac{a_{ml}\overline{a_{lj}}}{n} \langle \widetilde{\sigma}_{-Q,i}\widetilde{\sigma}_{Q,j} \rangle_{eq}. \tag{15}
$$

Here, the static correlation functions $\langle \widetilde{\sigma}_{-Q,i}\widetilde{\sigma}_{Q,l} \rangle_{eq}$ are given by

$$
\langle \widetilde{\sigma}_{-Q,i}\widetilde{\sigma}_{Q,l} \rangle_{eq} = \begin{cases}
\frac{1-u^{2n}}{1-2u^n \cos(nQ)+u^{2n}} & (i = l) \\
u^{|l-i|} \frac{e^{iQn} u^n}{1-e^{iQn} u^n} + u^{-|l-i|} \frac{e^{-iQn} u^n}{1-e^{-iQn} u^n} & (i \neq l) \\
\quad + u^{|l-i|}
\end{cases} \tag{16}
$$

while $u = \tanh(\frac{J}{k_BT})$, a_{ml} denotes the $(m,l)-$ element of the matrix $\mathbf{A}$ formed with the eigenvectors of $\mathbf{M}_Q$ and $\overline{a_{lj}}$ the $(l,j)-$ element of the matrix $\mathbf{A}^{-1}$. Finally, by using the fluctuation dissipation theorem[4], the response function $S_Q(\omega)$ turns out to be given by

$$
\begin{aligned}
S_Q(\omega) &= \frac{1}{k_BT}\left(\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\langle\widetilde{\sigma}_{-Q,i}\widetilde{\sigma}_{Q,l}\rangle_{eq} - i\omega\widetilde{C}_Q(\omega)\right) \\
&= -\frac{1}{k_BT}\sum_{l=1}^{n}\frac{\lambda_{lQ}g_{lQ}}{i\omega - \lambda_{lQ}}.
\end{aligned}
\tag{17}
$$

It should be noted that the frequency dependent susceptibility is $\chi(\omega) \equiv k_BTS_0(\omega)(1-u)/(1+u)$. Thus,

$$
\chi(\omega) = \frac{u-1}{u+1}\sum_{l=1}^{n}\frac{\lambda_{l0}g_{l0}}{i\omega - \lambda_{l0}}
\tag{18}
$$

If we set all the $\alpha's$ equal in Eq. (17), *i.e.*, we take the uniform chain, then of course the resulting susceptibility has the simple Debye form. In any case, its general structure is a linear combination of n Debye-like terms. In order to investigate whether the Nagel scaling holds for this susceptibility, it is convenient to recall that in the so-called Nagel plot 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 the susceptibility, W is the full width at half maximum of χ'', ω_p is the frequency corresponding to the peak in χ'', and $\Delta\chi = \chi(0) - \chi_\infty$ is the static susceptibility. For the sake of illustration in Figs. 1 and 2 we present Nagel plots for the cases $n = 2$ (with $\alpha_1 = 1$ and $\alpha_2 = 2$), and $n = 3$ (with $\alpha_1 = 1$ and $\alpha_2 = 2$ and $\alpha_3 = 3$), respectively, and different values of the reduced (dimensionless) temperature $T^* \equiv k_BT/2J$. By comparing the two figures, we can see that even for this case, where the relaxation times are very close, there is a marked improvement of the scaling in the low temperature limit with the increase of the relaxation mechanisms. On the other hand, the Debye scaling, shown as inset in the figures, presents an opposite behaviour. This result gives further support to the hypothesis that Nagel scaling is related to multiple relaxation mechanisms, as discussed in our previous work [2].
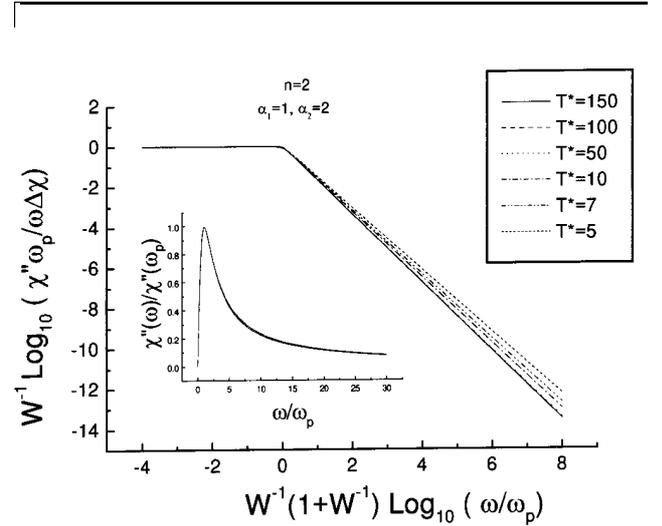
Figure 1. Nagel plot for $n = 2$ (with $\alpha_1 = 1$ and $\alpha_2 = 2$) and for $T^* = 5, 7, 10, 50, 100$ and 150. There is reasonable agreement with the scaling form for this choice except for low T^*. Insert: $\chi''(\omega)/\chi''(\omega_p)$ vs. ω/ω_p in order to test Debye-like behavior.
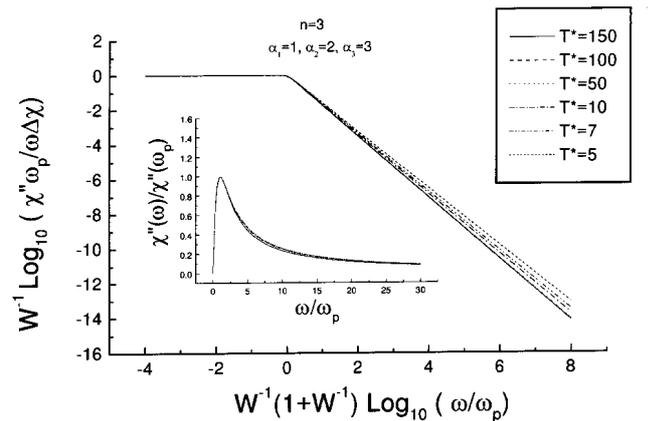

Figure 2. The same as Fig. 1 but with $n = 3$ ($\alpha_1 = 1$, $\alpha_2 = 2$ and $\alpha_3 = 3$) and $T^* = 5, 7, 10, 50, 100$ and 150. The improvement in the agreement with Nagel scaling is rather noticeable, while the opposite trend is observed with respect to Debye scaling.

References

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