5-20-1992

Thermal Rounding of the Charge Density Wave Depinning Transition

Alan Middleton
Syracuse University

Thermal Rounding of the Charge Density Wave Depinning Transition

A. Alan Middleton

Physics Department, Syracuse University, Syracuse, NY 13244

(Received)

The rounding of the charge density wave depinning transition by thermal noise is examined. Hops by localized modes over small barriers trigger "avalanches", resulting in a creep velocity much larger than that expected from comparing thermal energies with typical barriers. For a field equal to the $T = 0$ depinning field, the creep velocity is predicted to have a *power-law* dependence on the temperature T; numerical computations confirm this result. The predicted order of magnitude of the thermal rounding of the depinning transition is consistent with rounding seen in experiment.

Typeset Using *REVTEX*

The model [1] of an incommensurate charge density wave (CDW) as a deformable medium has been successful in explaining many experimental results both qualitatively and quantitatively [2]. In this model, the CDW is an elastic medium subject both to impurity pinning forces and an external drive force. At zero temperature, there is a sharp depinning transition: when the applied electric field E exceeds a threshold value E_T, the CDW depins, and the sliding CDW carries an electric current $j_{\rm CDW}$. Fisher [3] has proposed that the behavior near the depinning transition can be understood as a type of dynamic critical phenomenon. In particular, the CDW current $j_{\rm CDW}$ should behave as $j_{\rm CDW} \sim (E - E_T)^{\zeta}$, with ζ a critical exponent. Numerical work [4] has confirmed aspects of this picture in finite-dimensional models, and values for the exponent ζ have been determined [5,6].

This same numerical work has shown that, in order to clearly see the dynamic critical behavior, it is necessary to examine fields within a few percent of the depinning field E_T. It has proven difficult to obtain clear experimental results for applied fields this near to the depinning transition. A major cause of this difficulty is that the transition between the pinned and sliding state is not perfectly sharp [7] ; there is an apparent rounding in the $j_{\rm CDW}(E)$ relationship. Besides affecting the measurement of currents for E near E_T, the rounding makes it difficult to determine the threshold field E_T accurately. In order to make a careful comparison between experiment and theory, it is necessary to understand the rounding of the depinning transition.

Various explanations for this rounding have been proposed. One possibility is that experimental samples are macroscopically inhomogeneous, with local regions depinning at distinct applied fields E. The bulk $j_{\rm CDW}(E)$ relation would then be smeared. However, the sharp narrow band noise seen in many samples [2], indicates that the whole CDW is sliding at a uniform rate (though the narrow band noise is a finite size effect, its presence in finite experimental samples indicates uniform velocity). A somewhat related explanation is that provided by phase slip [8] in macroscopically homogeneous samples. Coppersmith has shown [9] that there exist exponentially rare regions with atypically weak pinning. Phase slip occurring on the border of such regions allows for an excess current below the bulk depinning field E_T. The main difficulty in attributing the rounding of the transition to this effect is the rarity of these atypical regions [10]. In particular, the magnitude of this effect will decrease as the exponential of a negative power of the impurity concentration. It has also been proposed [7] that thermal noise may round the CDW depinning transition.

In this paper, I examine the effects of finite temperature T on the CDW depinning transition. Recent work [11] has examined thermal effects at small field, far from the transition, where a creep velocity $\propto \exp[(ET)^{-\mu}]$ is expected, for some exponent μ. I study here instead the thermal effects at fields $E \approx E_T$, by examining the barriers that prevent the forward motion of Lee-Rice domains (regions of a size such that pinning and elastic forces are comparable and that act roughly as single degrees of freedom [1]). At first sight, thermal effects in CDW's might be expected to be very small, since the thermal energies are $\sim 10^3 - 10^7$ times smaller than the typical barrier energies estimated from the magnitude of the threshold field. This is consistent with the thermal creep for small fields, $E \ll E_T$, being extremely small. However, at $T = 0$, for fields just below the depinning threshold, many of the barriers to forward motion are much smaller than the typical barriers [3,12]. If the field is increased slightly, the smallest barriers vanish, and spatially localized instabilities are induced, leading to the "jumping" forward of individual Lee-Rice domains. Numerical calculations at $T = 0$ for fields below threshold show that the jumping forward of a single domain may cause an "avalanche", in which a large region of the CDW slides forward, as shown in Refs. [5,6]. At fields just above threshold, there is no stable configuration, and these triggering jumps and resulting avalanches lead to a positive CDW velocity. The argument I develop here estimates the current induced by the inclusion of thermal noise, which causes "hops" with effects similar to those due to the "jumps" resulting from an increase in field. These "hops" result in avalanches, as shown in Fig. 1. For $E = E_T$, this argument results in a prediction for the CDW velocity (directly proportional to the current j_{CDW}) of the form

$$v(T, E = E_T) \sim T^{\zeta/\tau}, \tag{1}$$

where τ is a non-universal exponent, with the values $\tau = 3/2$ for the usual Fukuyama-Lee-

Rice model, and $\tau = 2$ for a "ratcheted-kick" model [5]. The form of this scaling (with $\tau = 3/2$) is the same as that predicted by Fisher in mean field theory using a related, but distinct, argument [3]. I find the power law behavior (1) to be consistent with numerical results in dimensions $d = 2, 3$. For thermal energies on the order of 10^{-4} of the typical barrier height, these numerical calculations show a broadening of the transition on the order of 0.5%, in $d = 2, 3$, in order of magnitude agreement with experimental observations.

The Fukuyama-Lee-Rice model Hamiltonian [1] on a cubic (or square) lattice in scaled units is given by [4,14,12]:

$$\mathcal{H} = \frac{1}{2}\sum_{\langle ij\rangle}(\phi_i - \phi_j)^2 + h\sum_i V(\phi_i - \beta_i) - E\sum_i \phi_i, \tag{2}$$

where ϕ_i is the CDW phase at spatial site i, h is the impurity pinning strength, β_i is a random pinning phase, uniformly chosen in the interval $[0, 2\pi)$, and $V(\phi - \beta)$ gives the shape of the pinning potential. The first term of Eq. (2) represents elastic interactions between nearest neighbor pairs of sites $\langle ij\rangle$, the second term models pinning by impurities, and the last term represents the CDW polarization energy. I consider here two potentials V: the usual, smooth potential $V = \cos(\phi_i - \beta_i)$ and a sharp "ratcheted-kick" potential [5], which is, effectively, a sawtooth function of $\phi_i - \beta_i$. Evolution of the ϕ_i in time t is given by overdamped equations of motion $d\phi_i/dt = -(\partial\mathcal{H}/\partial\phi_i) + \eta_i(t)$, with Langevin noise $\eta_i(t)$, $\langle\eta_i(t)\eta_i(t')\rangle = 4TE_T\delta(t-t')$, so that temperature T is measured in units of the barrier energy scale $2E_T$ set by the threshold field. For $T = 0$, the velocity $v = \langle d\phi_i/dt\rangle_i$ is zero for $|E| \leq E_T$ and is positive for $E > E_T$, with $v \sim f^\zeta$ for small reduced field $f \equiv (E - E_T)/E_T$. As there is no phase slip in this model, the temporally averaged velocity must be uniform throughout the system, and there is a *single* threshold field at $T = 0$. For $|E| < E_T$, the polarization is defined as $P \equiv \langle\phi_i\rangle$. Numerical investigation of the sub-threshold state [5,12,13] shows that the *linear* polarizability of the CDW can be understood as the sum of contributions from spatially localized modes. As the applied field is increased, the modes with the smallest linear relaxation rates become unstable (via a saddle-node bifurcation), resulting in localized, irreversible jumps in the CDW phase. These jumps trigger avalanches over regions which become larger as threshold is approached; these jump and avalanche combinations are the dominant contribution to the *nonlinear* polarizability of the CDW [5].

Consider the CDW configuration $\{\phi_i\}$ at the threshold field, $E = E_T$, and temperature $T = 0$. The localized modes of the CDW configuration can be considered as (linearly) independent degrees of freedom ψ_k (k being mode indices), each with size approximately that of a Lee-Rice domain. Each ψ_k sees an individual potential $W_k(\psi_k)$, due to elastic, pinning, and drive forces, with $\sum W_k(\psi_k) = \mathcal{H}$. When the CDW is in a stationary configuration, each ψ_k is at a local minimum of W_k. Expanding W_k in powers of ψ_k, with $\psi_k \equiv 0$ at the inflection point separating the local minimum from the barrier to forward motion, gives (see also Refs. [3,4]):

$$W(\psi_k) = \frac{1}{3}A\psi_k^3 + B_k\psi_k - (\chi_k + 1)(E - E_T)\psi_k + O(\psi_k^5), \tag{3}$$

where A is approximately independent of k with a value determined by the strength and periodicity of the pinning potential and B_k and χ_k are positive; for the softest modes k, B_k approaches zero, while χ_k, which incorporates the linear polarizability of neighboring domains, is of order one. The potential $W(\psi_k)$ changes in response to an increase of the applied field. If E is increased by a small amount δE, minima of the local potentials vanish where B_k is smaller than $\delta E/(\chi_k + 1)$. As a result, some ψ_k jump forward and trigger an avalanche. By *destabilizing* a local mode, the increase of the field E leads to a current pulse. I now argue that, using Eq. (3), the effects of hops caused by a finite temperature can be directly related to the effects of the field induced destabilization of local modes.

It is useful to note two numerical results from $T = 0$ simulations of CDW's in finite dimensions: the apparent insensitivity of the exponent ζ to the shape of the pinning potential and the relatively quick relaxation of the velocity in the moving state. In the rather different cases of the smooth pinning potential and the ratcheted-kick potential, ζ is found to be universal to within numerical error, for $d = 2$, even though the mean-field exponents are distinct. The difference in the mean-field critical behavior of the two models results from the details of how a jump occurs. The apparent universality of ζ therefore suggests that the details of *how* a single domain jumps is unimportant in determining the critical behavior of the velocity in finite-dimensional models. This conclusion is supported by the observation that the velocity equilibrates well before the configuration reaches a periodic state. These numerical observations imply that the velocity is dominated by the avalanches which are triggered by the jumps, with the critical behavior of the velocity independent of jump dynamics and the shape of the sliding configuration.

These results suggest that thermally-induced hopping over small barriers will have the same effect on the velocity as raising the applied field by an amount which causes the destabilization of the same soft modes, if the time scale for the hop is much smaller than that for the evolution of the resulting avalanche. For potentials of the form Eq. (3), the barrier height Δ_k behaves as $\Delta_k \sim B_k^{3/2}$. Since a finite temperature T will cause rapid tunneling over barriers of height $\Delta_k \approx T$, thermal noise triggers avalanches at a rate corresponding to an applied field E with $(E - E_T) \sim T^{2/3}$, assuming χ_k of order one [15]. It follows that, for small T at an applied field $E = E_T$, the velocity v, due to avalanches triggered by thermal noise, scales as $v \sim T^{\zeta/\tau}$, where the exponent $\tau = 3/2$. For the case where pinning potential $V(\phi - \beta)$ is given by the ratcheted-kick form, it can be similarly shown that $\tau = 2$. Thermal effects are therefore non-universal in the shape of the pinning potential (it is probable however that the thermal effects *are* universal if the noise is due to finite random kicks, rather than Langevin noise [5]). The comparison of the effects of small reduced fields f and temperature T also suggests the scaling form

$$v(f, T) = T^{\zeta/\tau}\overline{B}(fT^{-1/\tau}), \tag{4}$$

which is exactly the form proposed by Fisher for mean-field theory [3], with $\overline{B}(u)$ behaving as u^{ζ} for large positive u and decaying very rapidly as $u \to -\infty$.

I have used numerical simulations for dimensions $d = 2, 3$ to check the scaling behavior predicted by Eqs. (1,4). The pinning strength $h = (2.5)d$ is chosen so that the size of a Lee-Rice domain is approximately one lattice unit. The computations were performed on a Connection Machine CM-2, utilizing 16K processors for approximately 35h.

Fig. 2 shows velocity v as a function of dimensionless temperature T on a log-log scale, for fixed field $E = E_T$ and a smooth potential V. The straight lines shown are not fits to the data, but have slopes predicted by Eq. (1) with values for the dynamical exponent of [5,6] $\zeta = 0.63, 0.85$ in $d = 2, 3$, respectively (estimated error bars for ζ in $d = 2, 3$ are 0.07; the value for ζ in $d = 3$ is from simulations on the ratcheted-kick model), and the predicted exponent $\tau = 3/2$. There is very good agreement between the data and Eq. (1), for velocities $v \lesssim 0.1$ (this velocity scale corresponds to the crossover between the high field and critical behavior in $T = 0$ simulations [5].) If the slope is allowed to vary, a best fit yields $\zeta/\tau = 0.40 \pm 0.04, 0.60 \pm 0.06$ in $d = 2, 3$, respectively. Similar calculations for the "ratcheted-kick" model in $d = 2, 3$ also show power-law behavior consistent with (1), for the above values of ζ, but with $\tau = 2$. It follows that the relationship between v and $k_B T/h$ is non-universal; this is not surprising given the derivation of Eq. (1), which, when Langevin noise is used, depends on microscopic properties of the model.

In order to examine the (non-universal) scaling function $\overline{B}$ of Eq. (4) for a particular case, velocities have also been calculated for fixed temperature and varying field. In Fig. (3), scaled velocity $vT^{-\zeta/\tau}$ is plotted as a function of scaled reduced field $fT^{-1/\tau}$ for the smooth pinning potential in $d = 2$, for the above values of ζ and τ. The scaling form Eq. (4) describes the data well. If ζ and τ are allowed to vary so as to produce the best fit to a single curve, I find $\zeta = 0.6 \pm 0.1$ and $\tau = 1.6 \pm 0.2$ (with subjective error bars). For dimensionless temperatures T of order 10^{-4}, this plot indicates that the rounding of the transition occurs over a range of $\sim 1\%$ in reduced field, in $d = 2$. In general, the width in field E of the rounding of the v vs. E curve, will be some constant times $E_T T^{1/\tau}$, independent of dimension. Using this criterion and the data of Fig. (2), the width of the rounding is found to be $\sim 0.5\%$ for $T = 10^{-4}$ in $d = 3$.

The scaling predictions of Eqs. (1,4), which are supported by these numerical simulations, can be directly applied to experiment. The temperature scale set by the typical barrier is of the order $E_B = 2\rho V_{\mathrm{FLR}} E_T \lambda_{\mathrm{CDW}}$, where λ_{CDW} is the wavelength of the CDW, which determines the periodicity of the pinning potential, ρ is the CDW charge density, and V_{FLR}

is the Fukuyama-Lee-Rice domain volume. For typical values of the parameters in $NbSe_3$ ($\lambda_{\rm CDW} = 4\AA$, $E_T = 100$ mV/cm, $\rho = 2\times 10^5$C/m^3, $V_{\rm FLR} = (0.1\mu{\rm m})^3$), at 125K, the dimensionless temperature is $T = 3\times 10^{-5}$, on the order of the smallest temperatures examined in the simulations reported here, so that the rounding in this case should be on the order of 1%. Generally, the materials parameters, such as the elastic constant (which affects $\xi_{\rm FLR}$) and charge density, are strongly dependent on temperature, making it quite difficult to verify the scaling predictions by comparing with experiments where the physical temperature is varied. The most direct method for checking the behaviors in Eqs. (1,4) may be to control the *dimensionless* temperature by varying the concentration of weak pinning impurities. For weak pinning, with impurity concentration n_i, the dimensionless temperature $T \propto E_B^{-1} \propto n_i^{(2-d)/(d-4)}$ [1,2].

I am pleased to acknowledge discussions with D. S. Fisher, P. B. Littlewood, J. Sethna, and C. Myers. The computational work was conducted using the resources of the Northeast Parallel Architectures Center (NPAC) at Syracuse University.

REFERENCES

[1] H. Fukuyama and P. A. Lee, Phys. Rev. B **17**, 535 (1977); P. A. Lee and T. M. Rice, Phys. Rev. B **19**, 3970 (1979); K. B. Efetov and A. I. Larkin, Sov. Phys. JETP **45**, 1236 (1977); L. Sneddon, M. C. Cross and D. S. Fisher, Phys. Rev. Lett. **49**, 292 (1982).

[2] For reviews, see *Charge Density Waves in Solids*, edited by L. P. Gorkov and G. Grüner (Elsevier, 1989); G. Grüner, Rev. Mod. Phys. **60**, 1129 (1988).

[3] D. S. Fisher, Phys. Rev. Lett. **50**, 1486 (1983); Phys. Rev. B **31**, 1396 (1985).

[4] For a review of numerical work, see P. B. Littlewood, in [2].

[5] A. A. Middleton and D. S. Fisher, Phys. Rev. Lett. **66**, 92 (1991); A. A. Middleton, Princeton University thesis, 1990 (unpublished); D. S. Fisher and A. A. Middleton, to be published.

[6] C. Myers and J. Sethna, to be published.

[7] M. O. Robbins, J. P. Stokes, and S. Bhattacharya, Phys. Rev. Lett. **55**, 2823 (1985); S. Bhattacharya, M. J. Higgins and J. D. Stokes, Phys. Rev. Lett. **63**, 1503 (1989); J. McCarten, *et al*, Phys. Rev. B **43**, 6800 (1991).

[8] M. Inui and S. Doniach, Phys. Rev. B **35**, 6244 (1987); S. H. Strogatz, C. M. Marcus, R. M. Westervelt, and R. E. Mirollo, Phys. Rev. Lett. **61**, 2380 (1988).

[9] S. Coppersmith, Phys. Rev. Lett. **65**, 1044 (1990); S. Coppersmith, to be published.

[10] If a large part of the current is due to tearing of the CDW, this should also be apparent in the relation between the narrow-band-noise frequency and the CDW current, which is linear when the CDW slides as a whole.

[11] P. B. Littlewood and R. Rammal, Phys. Rev. B **38**, 2675 (1988); T. Natterman, Phys. Rev. Lett. **64**, 2454 (1990); J. Toner, Phys. Rev. Lett. **64**, 2537 (1991).

[12] P. B. Littlewood, Phys. Rev. B **33**, 6694 (1986); P. Sibani and P. B. Littlewood, Phys. Rev. Lett. **64**, 1305 (1990).

[13] S. N. Coppersmith and D. S. Fisher, Phys. Rev. A **38**, 6338 (1988).

[14] L. Pietronero and S. Strassler, Phys. Rev. B **28**, 5863 (1983).

[15] For a mode ψ_k which becomes unstable at a field F_k, the eigenfrequency behaves as $\Lambda_k \sim (F - F_k)^\mu$, with μ apparently having the trivial value 1/2 [5,13], so that χ_k does not diverge as $F \nearrow F_k$.

FIGURES

FIG. 1. CDW velocity v vs. time t for a 128^2 sample, with $(E - E_T)/E_T = 0.98$ and $T = 10^{-5}$ in dimensionless units. Noise-triggered avalanches are visible above the local thermal fluctuations. The inset shows the avalanches which occur in the interval between the two arrows; dark regions show where the phase ϕ_i advances by more than π. In most of the volume of the avalanches, the phase advances by an amount close to 2π, while in the light regions, the phase changes by much less than 1.

FIG. 2. Plot of CDW velocity v as a function of dimensionless temperature T at the threshold field E_T, with smooth pinning potential. The key indicates the sample size and number of samples averaged over. The lines show slopes given by ζ/τ for exponent values given in the text for $d = 2$ (dashed) and $d = 3$ (dotted).

FIG. 3. Thermal rounding of the depinning transition for $d = 2$ with smooth potential: symbols show scaled velocity $vT^{-\zeta/\tau}$ vs. scaled reduced field $fT^{-1/\tau}$ for two different temperatures, using $\tau = 1.5$ and $\zeta = 0.63$. The solid line shows power law behavior $v \sim f^{\zeta}$, which determines the scaling function $\overline{B}$ in the large $fT^{-1/\tau}$ limit.

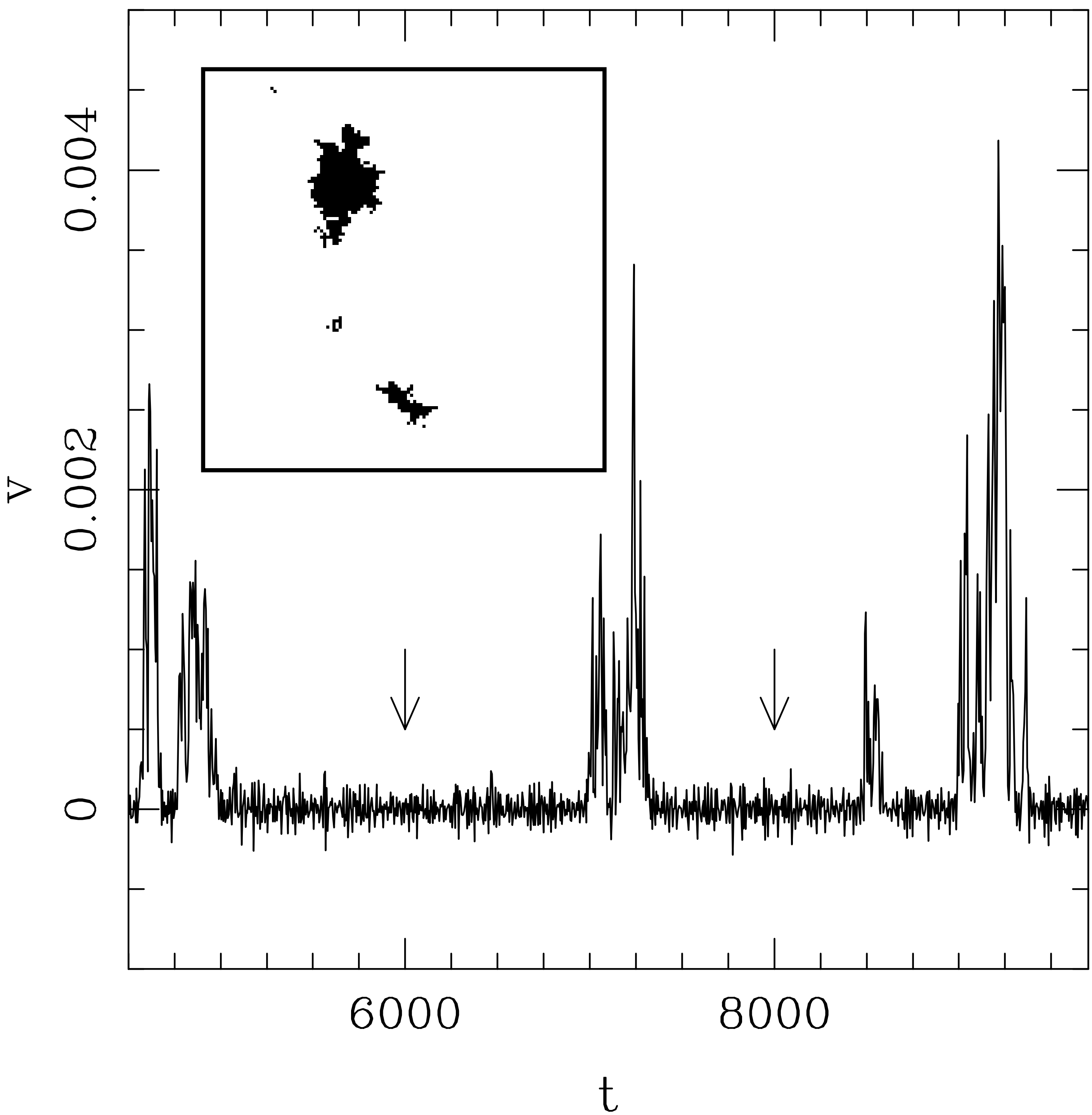

Fig. 1 - A. A. Middleton, "Thermal Rounding ..."

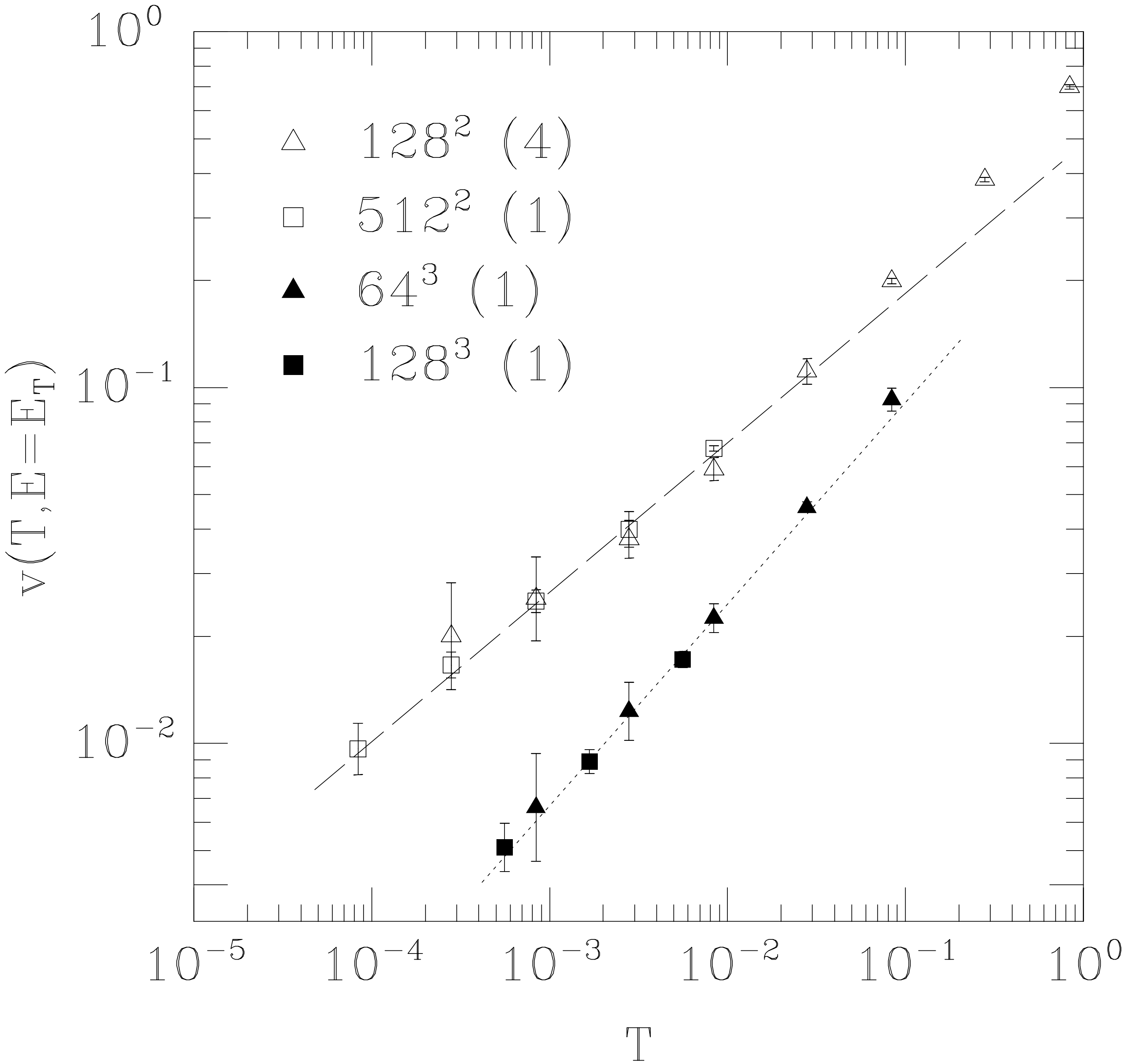

Fig. 2 - A. A. Middleton, "Thermal Rounding ..."

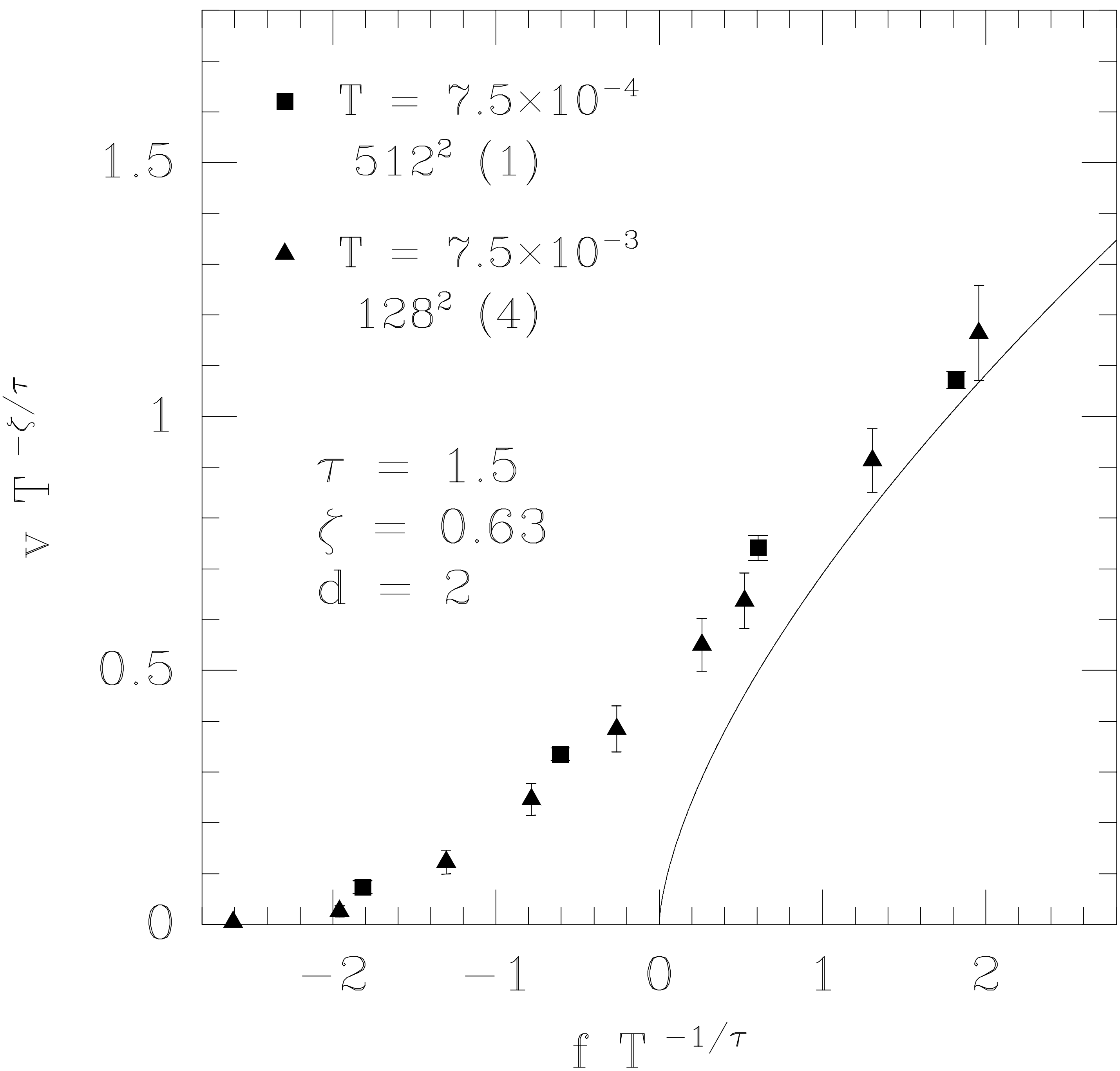

Fig. 3 - A. A. Middleton, "Thermal Rounding ..."