Tunneling Levels and Specific Heat of One-Dimensional Chaotic Configurations

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For a translationally invariant model of a chain of classical particles with competing interactions, the existence of tunneling levels is proved. Their density of states, which exhibits a scaling property, is derived for a special type of quenched disorder. Finally it is shown that the low-temperature specific heat behaves like $c(T) \sim T^{\tilde{d}}$ with a fractional exponent $\tilde{d} = -(\ln 2)/\ln|\eta| < 1$, where η depends on the coupling constants.

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The linear temperature dependence of the specific heat $c(T)$ of amorphous solids below 1 K found experimentally[1] and explained[2,3] by the existence of tunneling levels with constant density of states on the scale of 10^{-5}–10^{-4} eV is rather exceptional. For instance, for vitreous Se a $T^{0.5}$ law was found.[4] In the meantime, several experiments have confirmed such fractional exponents.[5]

In this Letter, I present two main results: (i) For a chain of classical particles with competing interactions the existence of two-level systems (TLS) is proved. Their density of states and the potential barriers are derived exactly. As far as I know[6] this was not done before. A qualitative approach was recently given by using topological arguments.[7]

(ii) For chaotic (amorphous) arrangements of the atoms, which do *not* have a fractal structure,[8] I show that, nevertheless, the TLS form a Cantor set with fractal dimension $\tilde{d}$.[8] This may explain the fractional exponents of $c(T)$ below 1 K. Similar Cantor spectra were recently found for the vibrational modes of fractals,[9–11] but because amorphous solids are not fractals, the results presented here seem more appealing.

Consider a chain of particles with interactions up to rth nearest neighbors,

$$V = \sum_n \sum_{l=1}^{r} V_l(u_{n+l} - u_n), \tag{1}$$

where V_l is the interaction energy between the lth nearest neighbors and u_n the position of the nth atom. ($r = 2$ is assumed in the following.) For the nearest-neighbor interaction, we use a double-well potential with minima at a_1 and a_2,

$$V_1(x) = \tfrac{1}{2} C_1 [x - a_+ - a_- \sigma(x)]^2, \quad C_1 > 0, \quad a_\pm = \tfrac{1}{2}(a_2 \pm a_1), \tag{2a}$$

where

$$\sigma(x) = \mathrm{sgn}(x - a_+), \tag{2b}$$

and a harmonic interaction for V_2,

$$V_2(x) = \tfrac{1}{2} C_2 (x - b)^2, \quad C_2 \geqslant 0. \tag{2c}$$

Similar exactly solvable models were used to study spatially modulated phases.[12,13] The presence of two degenerate energy minima of V_1 may also model two types of "molecules" with equilibrium size a_1 and a_2. The results presented in this Letter do not change much for more general, piecewise-parabolic potentials, e.g., those with only one minimum. This and details of the calculations presented here, as well as the investigation of the pair distribution function, will be discussed elsewhere.[14]

Under the assumption that the stress in the chain [which is an invariant because of the translational invariance of (1)] is zero and with the atomic distances

$$v_n = u_{n+1} - u_n,$$

the equation $(\partial V/\partial u_n) = 0$ for the equilibrium configurations reduces to

$$C_1(v_n - a_- \sigma_n) + C_2(2v_n + v_{n-1} + v_{n+1}) - a_+(C_1 + 2bC_2) = 0, \tag{3a}$$

where

$$\sigma_n = \sigma(v_n), \tag{3b}$$

and $\sigma_n = \pm 1$ because of (2b).

The bounded solutions of (3a) can be obtained, following Refs. 12 or 13, as

$$v_n = A + \tfrac{1}{2} B(1-\eta)(1+\eta)^{-1} \sum_{i=-\infty}^{\infty} \eta^{|i|} \sigma_{n-i}, \tag{4}$$

where

$$A=(1-\eta)^{-2}[(1+\eta)^2 a_+ - 2\eta b], \quad B=2a_-(1-\eta)^{-2}(1+\eta)^2,$$

$$\eta=-\gamma[1-(1-\gamma^{-2})^{1/2}], \quad \gamma=1+C_1/2C_2.$$

A configuration $v=\{v_n\}$ following from (4) by specifying a sequence $\sigma=\{\sigma_n\}$, $\sigma_n=\pm 1$, is an equilibrium configuration if and only if (i) v_n are positive and bounded and (ii) the self-consistency condition (3b) is fulfilled. It can be shown[14] that for $|\eta|<\frac{1}{3}$ there exists a finite range for (a_1,a_2,b) such that (i) and (ii) are satisfied for *any* sequence σ. In addition it is easy to prove (because of the piecewise-parabolic potential) that the metastability of *all* equilibrium configurations is guaranteed for $C_2>-\frac{1}{4}C_1$, i.e., $|\eta|<1$.

Equation (4) is an explicit example for an embedding of the Bernoulli shift justifying recent investigations[15] of chaotic configurations. Substitution of v_n from Eq. (4) into (2) yields the energy of the equilibrium configurations $v=\{v_n\}$,

$$E(v(\sigma))=e_0\sum_n 1+h\sum_n\sigma_n+\sum_{n\neq m}J(n-m)\sigma_n\sigma_m, \tag{5}$$

where

$$e_0=\alpha[(2a_+-b)^2+2a_-^2(1-\eta)], \quad h=\alpha 4a_-(2a_+-b),$$

$$J(m)=J_0\eta^{|m|}, \quad J_0=\alpha a_-^2(1-\eta^2)/\eta, \quad \alpha=C_2(1+\eta)^2/2(1-\eta)^2.$$

For a given sequence $\sigma=\{\sigma_n\}$, let $i-1$ and i be bonds with $\sigma_{i-1}=-1$ $(+1)$ and $\sigma_i=1$ (-1). A new metastable configuration $v(\sigma')$ with $\sigma'_{i-1}=\sigma_i$, $\sigma'_i=\sigma_{i-1}$, and $\sigma'_n=\sigma_n$ otherwise is obtained from $v(\sigma)$ just be moving the ith atom over a potential barrier and then relaxing the chain. From (5) we obtain the energy difference $E(v(\sigma'))-E(v(\sigma))=\epsilon_i(\sigma)$,

$$\epsilon_i(\sigma)=4J_0(1-\eta)\sum_{\nu=1}^{\infty}\eta^\nu(\sigma_{i-1-\nu}-\sigma_{i+\nu}). \tag{6}$$

By addition of an external force term $(-Fv_{i-1}-F'v_i)$ to (1), the equilibrium configurations can be calculated as a function of F and F' and the barriers Δ_i can be derived as

$$\Delta_i(v(\sigma))=-C_2(2\eta)^{-1}[(a_+-v_{i-1})^2-2\eta(a_+-v_{i-1})(a_+-v_i)+(a_+-v_i)^2] \tag{7}$$

which is positive because $|\eta|<\frac{1}{3}$ and $C_2/\eta<0$, independent of the sign of C_2. The energy differences [Eq. (6)] between two local minima are classical energies. At low temperatures the following quantum corrections may become important: (i) the zero point energy $\hbar\omega_i$ and (ii) a change of energy as a result of resonant tunneling. Using V_1 and V_2 [Eqs. (2a) and (2b)] we find that the zero-point energy is equal to $\hbar\omega_0=\hbar[-2C_2/(\eta m)]^{1/2}$ (m is the particle mass and remember $C_2/\eta<0$) for *all* local minima due to the special form of V_1. Thus the zero-point energies just cancel for the energy differences.

Using Eqs. (6) and (7) one can show that the correlations between $\epsilon_i(\sigma)$ and $\Delta_i(\sigma)$ become so weak for ϵ_i of the order 10^{-4} eV or smaller that they may be neglected. In addition, it can be shown that $\Delta_{\min}\leq\Delta_i\leq\Delta_{\max}$ for all i, with $\Delta_{\min}=(-C_2/\eta)a_-^2(1+\eta)^3$ and $\Delta_{\max}\leq 2\Delta_{\min}$ for all $|\eta|<\frac{1}{3}$.

Let us assume in the following that $\Delta_{\max}=0.1$ eV; thus $\Delta_{\min}\geq 0.05$ eV. Following Ref. 2 we determine $\lambda_{\min}$ and $\lambda_{\max}$ ($e^{-\lambda}$ is the overlap of the wave functions) for an oxygen atom and a separation of the potential wells equal to $a_-=1$ Å. The parameter $(-C_2)/\eta$ can be obtained from $\Delta_{\min}$ which then leads, for $\eta=\frac{1}{4}$, to $\hbar\omega_0\approx 2\times 10^{-3}$ eV and $\lambda_{\min}=\ln(2\hbar\omega_0/\epsilon_i)\leq 6$ ($\epsilon_i\geq 10^{-5}$ eV). For a specific-heat measurement with time scale $t=10$ sec it follows $\lambda_{\max}=\frac{1}{2}\ln\Gamma_0 t<16$ where we have assumed $\Gamma_0=\omega_0$ ($\Gamma=\Gamma_0 e^{-2\lambda}$ is the tunneling rate). From $\Delta_{\min}\leq\Delta_i\leq\Delta_{\max}$ we obtain that $9<\lambda_i<13$ for all i. Thus for all the potential barriers $\lambda_{\min}<\lambda_i<\lambda_{\max}$. $\lambda_i>\lambda_{\min}$ means that resonant tunneling can be neglected, i.e., the energies ϵ_i are, within this approximation, the tunneling levels, and $\lambda<\lambda_{\max}$ justifies taking all tunneling levels between 10^{-5} and 10^{-4} eV into account for the calculation of the specific heat.

Now we will specify σ which leads to chaotic configurations. Special chaotic (amorphous) arrangements of the atoms are obtained for sequences which are *normal*, i.e., sequences for which all the 2^k possible subsequences of length k occur with

equal probability 2^{-k} for all k (analogous to normal numbers[16]). Non-normal sequences of the form $\sigma_n = 1$ for $n \neq km$ and σ_n random ($= \pm 1$) for $n = km$, for a fixed integer k and all integers m, lead to chaotic but *microcrystalline structures.* The importance of normal numbers for amorphous configurations was also pointed out in Ref. 15. In the following the sequence σ, which characterizes the type of *quenched bond disorder,* is assumed to be normal.

The tunneling levels (6) form a Cantor spectrum with fractal dimension:

$$\hat{d} = -(\ln 3)/\ln|\eta|. \tag{8}$$

This property originates from the Cantor-set structure built by the nearest-neighbor distances (4) similar to results for a Frenkel-Kontorova-type model.[17]

The density of states $n(\epsilon)$ can be obtained as follows: For an energy resolution equal to $\epsilon_0|\eta|^\nu$ [$\epsilon_0 = 8|J_0\eta|(1-\eta)$] we find for the νth order density of states $n_\nu(\epsilon)$

$$n_\nu(\epsilon) = n_0 \begin{cases} 2^{\mu-\nu}(2|\eta|)^{-\nu}, & \epsilon \text{ in } I^{\mu}_{\mu_1\ldots\mu_\nu}, \\ 0, & \text{otherwise}, \end{cases} \tag{9}$$

where

$$I^{\mu}_{\mu_1\ldots\mu_\nu} = [\epsilon_0(\textstyle\sum_{i=1}^{\nu}\mu_i|\eta|^{i-1} - \delta_\nu), \\ \epsilon_0(\textstyle\sum_{i=1}^{\nu}\mu_i|\eta|^{i-1} + \delta_\nu)],$$

$$\mu_i = 0, \pm 1, \quad \delta_\nu = |\eta|^\nu/(1-|\eta|),$$

and μ is the number of μ_i which are zero. $n_0 = (1 - |\eta|)/4\epsilon_0$. Here we have taken into account that for N particles there are $2N/4 = N/2$ tunneling levels (σ normal). $n_\nu(\epsilon)$ is presented in Fig. 1 for $\nu = 1$, 2, and 3.

From Eq. (9) we find the scaling property

$$n_{\nu+1}(|\eta|\epsilon) = (2|\eta|)^{-1} n_\nu(\epsilon), \tag{10}$$

for $|\epsilon| \leq \epsilon_0(1-|\eta|)^{-1}$ and $\nu \geq 1$, which also becomes obvious from Fig. 1. The spectral dimension $\tilde{d}$ defined by[18]

$$n(\epsilon) \sim \epsilon^{\tilde{d}-1} \quad (\epsilon \to 0) \tag{11}$$

follows from (10) for $\nu \to \infty$,

$$\tilde{d} = -(\ln 2)/\ln|\eta| = \hat{d}(\ln 2)/\ln 3. \tag{12}$$

That such a relation must hold follows from the definition of the fractal dimension $\hat{d}$,[8] which also implies $\hat{d} < 1$ for a Cantor set on the real line. Using (11) and (12) we get for the temperature dependence of the specific heat

$$C(T) \sim T^{\tilde{d}}, \quad 0.1\ K < T < 1\ K,$$

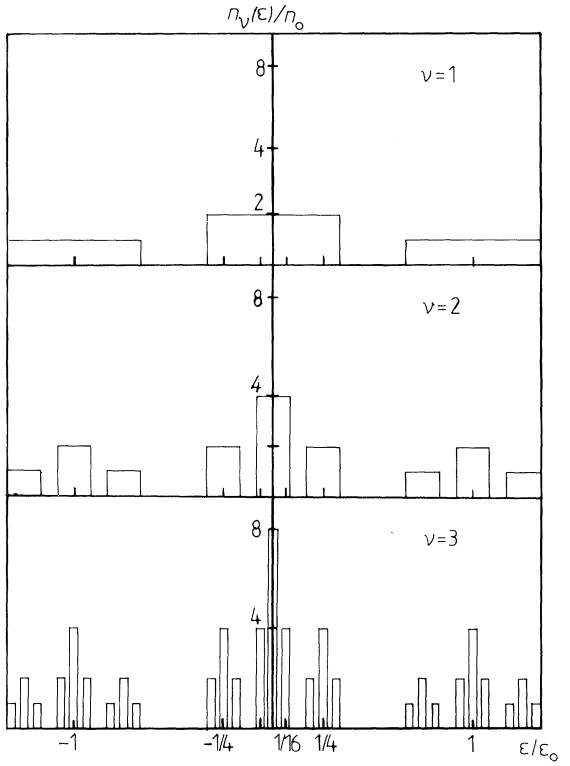

FIG. 1. The density of states $n_\nu(\epsilon)$ for $\nu = 1$, 2, and 3 and $|\eta| = \frac{1}{4}$.

with $\tilde{d}$ given by (12). Because $|\eta| < \frac{1}{3}$ it follows that $0 < \tilde{d} < 0.63$. Some experimental data, e.g., for Se,[4] are in that range. Fractional exponents larger[5] than 1 may also be possible for other models despite the fact that $\hat{d}$ is always less than 1. The gaps which exist in the spectrum of the tunneling levels (compare Fig. 1) may provide a microscopic justification of the phenomenological theory by Lasjaunias, Maynard, and Vandorpe.[19] With the assumption of a gap in the density of states, they obtained for the specific heat $c(T) \sim T^{1+\nu}$ with $0 < \nu < 1$.

In conclusion, the simple model studied here provides a microscopic derivation of tunneling levels and potential barriers. Both can be obtained for arbitrary quenched disorder because Eqs. (6) and (7) are true for any sequence σ. For a special class of disorder, which was given by normal sequences, the density of states is nonconstant and exhibits a scaling property as a result of the Cantor spectrum; this leads to a low-temperature specific heat $c(T) \sim T^{\tilde{d}}$, where $\tilde{d} < 1$ depends only on the ratio C_1/C_2 of the elastic constants. These results do not depend on the sign of C_2 and are stable against small anharmonic perturbations of $V_1(x)$, e.g., such as $C_1' x^4$ as

long as C_1' is small enough.[14]

The model I have studied may apply to quasi-one-dimensional systems or layered compounds. But it also seems possible that similar results may be true for two- and three-dimensional systems, because, for amorphous solids, the Euclidean dimension d does not play as important a role as in the Debye theory; instead $\tilde{d}$ may be the relevant quantity.

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