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Most probable paths in homogeneous and disordered lattices at finite temperature

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Abstract

We determine the geometrical properties of the most probable paths at finite temperatures T , between two points separated by a distance r , in one-dimensional lattices with positive energies of interaction ε_i associated with bond i . The most probable path-length t_{mp} in a homogeneous medium ($\varepsilon_i = \varepsilon$, for all i) is found to undergo a phase transition, from an optimal-like form ($t_{mp} \sim r$) at low temperatures to a random walk form ($t_{mp} \sim r^2$) near the critical temperature $T_c = \varepsilon/\ln 2$. At $T > T_c$ the most probable path-length diverges, discontinuously, for all finite endpoint separations greater than a particular value $r^*(T)$. In disordered lattices, with ε_i homogeneously distributed between $\varepsilon - \delta/2$ and $\varepsilon + \delta/2$, the random walk phase is absent, but a phase transition to diverging t_{mp} still takes place. Different disorder configurations have different transition points. A way to characterize the whole ensemble of disorder, for a given distribution, is suggested. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Consider a disordered lattice of bonds of random energy. A path along this lattice which minimizes the total energy is known as an *optimal path*. One may distinguish between two kinds of paths: paths of *fixed length*, and paths between two fixed endpoints but of *undetermined length*. The case of fixed length might be interpreted as a linear polymer that interacts strongly with a disordered surface or solvent; it has been studied in detail in the context of self-avoiding walks in random media [1–7]. Similarly, the case of undetermined length applies to a very long polymer that only portions of it

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interact with the substrate. Our study of optimal paths aims to elucidate how the length of the path depends on the end-to-end distance. The optimal path between two fixed points can be determined exactly by the Dijkstra algorithm [8]. Numerical studies by means of this technique show that the path length increases linearly with the distance between its endpoints, and therefore such paths are said to belong to the universality class of directed polymers [8,9].

The minimal energy sought by optimal paths corresponds to the limit of zero temperature. At finite temperature, there is no longer a unique path, due to thermal fluctuations, and instead we focus on the *most probable* path—in a thermodynamical sense. Most probable paths (at finite temperature) are markedly different from optimal paths (at zero temperature). For example, optimal paths are always self-avoiding, which is not necessarily true about most probable paths.

A useful representation of optimal, or most probable paths is achieved by augmenting the d -dimensional lattice with a perpendicular dimension along which the path evolves. This special dimension is referred to as “time”, t . Notice that the walk must always step forward in the t -direction (even in the case of finite temperature), so the path problem is recast into a directed walk in $d + 1$ dimensions (Fig. 1).

Directed paths at finite temperature have been studied only for the case of fixed length t [10,11]. A crossover was observed from random walk behavior, for small t ,

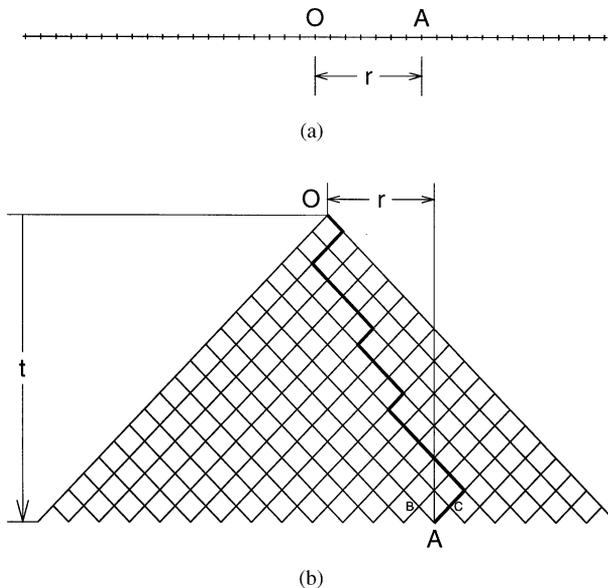


Fig. 1. (a) Two points, marked O and A, separated by r lattice units (or, bonds) on a one-dimensional lattice. A nondirected path of length t from O to A may be obtained by projecting on this lattice the directed path shown in part (b) of this figure. (b) A directed path (in bold line) of length t from O to A on a (1+1)-dimensional lattice. The horizontal dimension represents ‘space’ and the vertical dimension represents ‘time’. Directed paths on this lattice are those along which time can only increase. Any directed path from O to A is the resultant of adding either the bond BA to a directed path from O to B or the bond CA to a directed path from O to C. This is the basis of the iterative procedure stated in Eq. (14).

to optimal-like behavior, for large t . In other words, as long as t is large enough the behavior of directed polymers is the same as for optimal paths, regardless of the temperature.

In this paper, we address the problem of most probable paths of *undetermined length*, at finite temperature. The walks take place in a one-dimensional lattice, between two endpoints separated by a distance r (the length of the walks is $t \geq r$ not fixed). We first study an homogeneous lattice, where all the bonds have the same energy ε . This ostensibly simple case exhibits a surprisingly rich behavior. Given a distance r between the endpoints, there exists a critical temperature $T^*(r)$ such that the most probable length of the path, t_{mp} , is finite for $T < T^*(r)$, but infinite for $T > T^*(r)$. When t_{mp} exists ($T < T^*$), it exhibits crossover behavior; from $t_{mp} \sim r$ for small r , to $t_{mp} \sim r^2$ for large r . We then turn to disordered lattices, where the energy of a bond is in the range $(\varepsilon - \delta/2, \varepsilon + \delta/2)$, with uniform probability. In this case, the phase transition is somewhat modified: there is now a range of temperatures where a finite fraction of all disorder configurations possesses a well defined t_{mp} . Defining a critical temperature, $T_c(\varepsilon, \delta)$, as the temperature below which t_{mp} is finite for *all* configurations, we find that $T_c(\varepsilon, \delta) - T_c(\varepsilon, 0) \sim -\delta^x$, where $x \approx 1.2$.

2. Most probable paths in a homogeneous medium

2.1. Theory

Consider a one-dimensional chain where the energy associated with each bond is ε . The number $N(r, t)$ of all paths of length t , between two fixed points at distance r apart, is

$$N(r, t) = \binom{t}{\frac{t-r}{2}} = \frac{t!}{(t-r/2)!(t+r/2)!} \tag{1}$$

At temperature T each step on the lattice has a Boltzmann weight $e^{-\varepsilon/T}$ (we take $k_B = 1$); hence, each path of length t has a weight of $e^{-\varepsilon t/T}$. A “microcanonical” partition function, for paths of fixed length t , is

$$G_T(r, t) = N(r, t)e^{-\varepsilon t/T} \tag{2}$$

and the corresponding partition function, for paths of all possible lengths, is:

$$G_T(r) = \sum_t G_T(r, t) \tag{3}$$

Notice that there is no “chemical potential”, or “fugacity”. The length of our paths is controlled only by entropy and the energy of interaction with the lattice. The probability that the length of the path between the two fixed points is t , is

$$P_T(r, t) = \frac{G_T(r, t)}{G_T(r)} \tag{4}$$

The most probable path-length, t_{mp} , is the value of t for which $P_T(r, t)$ (or $G_T(r, t)$) is maximum. At $T = 0$, the only possible path is the optimal path, the one of minimal energy. In one-dimension it is simply the line joining the endpoints:

$$t_{mp}(r)|_{T=0} = r. \tag{5}$$

For $T > 0$, we assume $t \gg r$ and make use of Stirling’s approximation, to yield

$$G_T(r, t) \approx \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{t\varepsilon}{T} + (t + 1) \ln 2 - \frac{1}{2} \ln t - \frac{r^2}{2t} \right]. \tag{6}$$

Thus, from $dG_T(r, t)/dt|_{t_{mp}} = 0$, we find

$$t_{mp} = \frac{1 - \sqrt{1 - 8(\ln 2 - \varepsilon/T)r^2}}{4(\ln 2 - \varepsilon/T)}. \tag{7}$$

There emerge two different regimes:

(i) $\varepsilon/T > \ln 2$. In this case t_{mp} is well defined for all r . We identify two asymptotic behaviors, depending on whether the end-to-end distance r is smaller or larger than the crossover distance $r_\times = (\varepsilon/T - \ln 2)^{-1/2}$. For $r \ll r_\times$, we have

$$t_{mp} \approx r^2, \tag{8}$$

which is the signature of a random walk. Whereas for $r \gg r_\times$,

$$t_{mp} \approx \frac{r}{\sqrt{2(\varepsilon/T - \ln 2)}}, \tag{9}$$

similar to the linear relation characteristic of optimal paths at zero temperature. Note that the region where t_{mp} behaves like a random walk vanishes as $T \rightarrow 0$.¹

The asymptotic behavior may be summarized by the scaling form

$$t_{mp} = r^2 f \left(\frac{r}{r_\times} \right), \quad f(x) \sim \begin{cases} 1, & x \ll 1, \\ \frac{1}{\sqrt{2x}}, & x \gg 1. \end{cases} \tag{10}$$

(ii) $\varepsilon/T < \ln 2$. In this case, for every finite r there exists a temperature $T^*(r)$ such that t_{mp} is finite if $T < T^*(r)$, but infinite if $T > T^*(r)$:

$$T^*(r) = \frac{\varepsilon}{\ln 2 - 1/8r^2}. \tag{11}$$

Note that $T_c \equiv \lim_{r \rightarrow \infty} T^*(r) = \varepsilon/\ln 2$ might be thought of as a critical temperature, since for $T < T_c$ the most probable length is finite for *all* values of r . Conversely, for $T > T_c$, there exists a finite crossover distance

$$r^*(T) = \frac{1}{2\sqrt{2}} \left(\ln 2 - \frac{\varepsilon}{T} \right)^{-1/2}, \tag{12}$$

such that t_{mp} is well defined only for $r < r^*(T)$. Hence, at T_c both r_\times and r^* diverge, with the same critical exponent, $\nu = \frac{1}{2}$. The critical point at T_c can be further illustrated by the behavior of the *average* length of the paths, $\langle t \rangle$, which is finite for $T < T_c$ but infinite for $T > T_c$, regardless of r .

¹ For very low temperatures, $\varepsilon/T \gg \ln 2$, we have $t_{mp} \approx \sqrt{T/2\varepsilon}r$, which reproduces the expected optimal-like linear dependence of t_{mp} on r . The coefficient of r is however, incorrect because the necessary condition for the use of Stirling’s approximation, $t_{mp} \gg r$, is violated.

2.2. Numerical results

In the above discussion we have replaced factorials by the first term of Sterling's approximation, thus our results are applicable only for large r and t . For unrestricted values of r and t , analytic calculations may be easily carried out to any desired accuracy. Instead, we now describe a numerical iterative procedure that we also use for the study of disordered lattices. The results for homogeneous lattices presented in this section help validate the technique.

Consider a one-dimensional lattice with energies ε_i , associated with bond i . (The energy values are fixed, so in the 1 + 1-dimensional lattice of Fig. 1b the energies of the bonds in a given column are all the same.) The partition function for walks from $(0, 0)$ to (r, t) , at temperature T , is

$$G_T(r, t) = \sum_{\mathcal{C}} e^{-E_{\mathcal{C}}/T}, \quad (13)$$

where \mathcal{C} denotes a path from 0 to r of exactly t steps, i.e., a directed path from $(0, 0)$ to (r, t) . The energy of interaction of a path, $E_{\mathcal{C}}$, is the sum of the energies of the lattice bonds encountered along the path. The partition function follows the recursion relation [12]:

$$G_T(r, t + 1) = G_T(r - 1, t)e^{-\varepsilon_L/T} + G_T(r + 1, t)e^{-\varepsilon_R/T}. \quad (14)$$

where ε_L and ε_R are the energies of the bonds from $(r - 1, t)$ to $(r, t + 1)$ and from $(r + 1, t)$ to $(r, t + 1)$, respectively. This can be most clearly seen with help of Fig. 1b. In practice, however, only the one-dimensional array of $G_T(r, t)$, $-L \leq r \leq L$, is stored in the computer, and successive iterations for increasing values of t (starting with $G_T(r, 0) = \delta_{0,r}$) are generated by the exact enumeration method [13].

For the homogeneous lattice case, we take $\varepsilon_i = 1$, and we have used $L = 1000$. For each value of $r > 0$ and fixed temperature T the most probable path-length t_{mp} was identified as the value of t ($t < L$) for which $G_T(r, t)$ is maximum. At every temperature T , it was observed that beyond a certain value of r , $G_T(r, t)$ was maximum only at $t = L$, which means that t_{mp} could not be obtained within the finite lattice imposed.

The results obtained for t_{mp} as a function of r at various temperatures are shown in Figs. 2 and 3. Fig. 2a shows that the nature of the most probable path-length is almost entirely optimal-like ($t_{mp} \sim r$) for $T \ll 1/\ln 2$, but the random walk nature ($t_{mp} \sim r^2$) appears over a rapidly increasing range of r as $T \rightarrow 1/\ln 2 \approx 1.44269$. When the variables t_{mp} and r are rescaled according to Eq. (10), the data for different temperatures are seen to fall on a single curve, except for the region of very small r (Fig. 2b); this curve represents the universal scaling function $f(x)$ of Eq. (10). For $r \lesssim 8$ there is a large deviation from the scaling form due to the discreteness of the lattice.

The data for t_{mp} at temperatures above T_c are shown in Fig. 3a. In concurrence with the theoretical expectations, the random walk nature ($t_{mp} \sim r^2$) is evident at small values of r and eventually t_{mp} appears to diverge at a certain separation $r^*(T)$ for every temperature $T > 1/\ln 2$; at $r^*(T)$ we observe that the value of t_{mp} suddenly jumps to L .

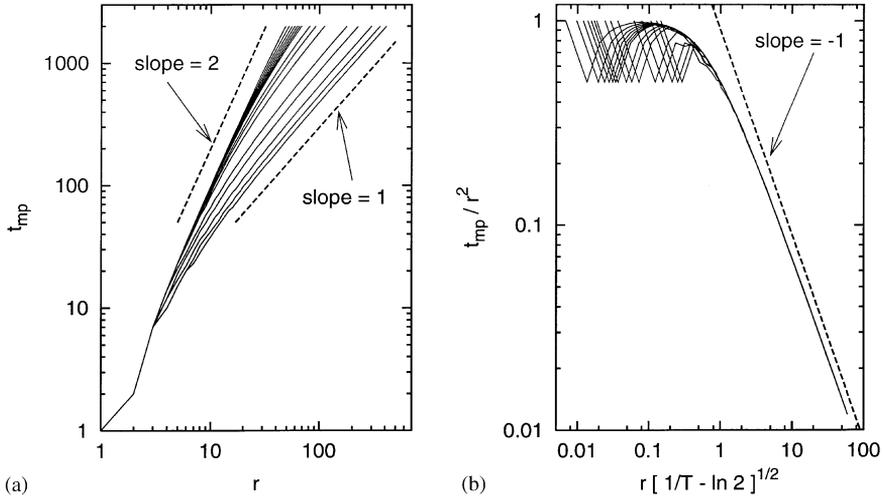


Fig. 2. (a) Most probable path-length t_{mp} as a function of the endpoint separation r at temperatures $T < T_c$ in a homogeneous medium. The curves, from right to left, are for the temperatures: 1.4, 1.41, 1.42, 1.43, 1.435, 1.44, 1.441, 1.442, 1.4421, 1.4422, 1.4423, 1.4424, 1.4425 and 1.4426. The data show that most probable paths far from $T_c = 1/\ln 2 \approx 1.44269$ are optimal-like ($t_{mp} \sim r$), indicated by the slope 1, whereas close to T_c the most probable paths are random walk-like ($t_{mp} \sim r^2$), indicated by the slope 2. (b) The curves for different temperatures collapse to a single curve when the data shown in part (a) of the figure are plotted with rescaled variables. The single curve is the universal scaling function of Eq. (10).

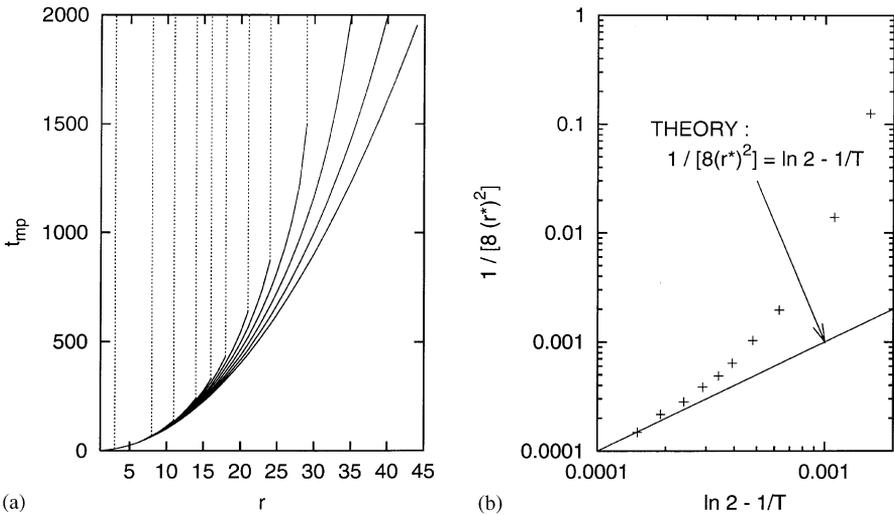


Fig. 3. (a) Most probable path-length t_{mp} as a function of the endpoint separation r , at temperature $T > T_c$, in a homogeneous medium. The curves, from right to left, are for $T = 1.4427, 1.4428, 1.4429, 1.443, 1.4431, 1.4432, 1.4433, 1.4434, 1.4435, 1.4437, 1.444$ and 1.445 . The curves for all the temperatures follow the parabola $t_{mp} = r^2$ for small values of r , but eventually separate out and diverge at a particular endpoint separation $r^*(T)$ characteristic of each temperature. The last curve on the right, which is the data for $T = 1.4427$, is closest to $T_c = 1/\ln 2 \approx 1.44269$ and it has the parabolic form almost throughout. (b) The characteristic endpoint separations $r^*(T)$ is shown as a function of the temperature T .

Fig. 3b shows the variation of r^* with temperature, which agrees well with the result derived from Sterling’s approximation as $T \rightarrow T_c$.

3. Most probable paths in disordered media

For the study of most probable paths in disordered lattices, we consider a lattice with random bond energies, ε_i , homogeneously distributed in $(\varepsilon - \delta/2, \varepsilon + \delta/2)$, where δ can be thought of as the parameter characterizing disorder: the limit $\delta \rightarrow 0$ corresponds to the homogeneous lattice. Furthermore, for comparison with the homogeneous results presented so far, we take $\varepsilon = 1$.

We have performed computer simulations of 10^4 realizations of disorder, for several ranges δ of energies, in one-dimensional lattices of 4000 bonds. For each realization of disorder the partition function $G(r, t)$ was calculated by the exact enumeration method of the previous section.

Unlike what is observed in a homogeneous medium, the random walk behavior of the most probable path-length never appears in the disordered case. Otherwise, a transition similar to that of the homogeneous case is observed, but with some features that are unique to disorder. For each realization, and for $T > T'$, there exist a $r^*(T)$ such that the most probable path-length diverges for endpoint separations $r > r^*(T)$. If $T < T'$, there is no divergence, regardless of r . An example, for a typical realization with $0.5 \leq \varepsilon_i \leq 1.5$ ($\delta = 0.5$), is shown in Fig. 4. In contrast to the homogeneous case,

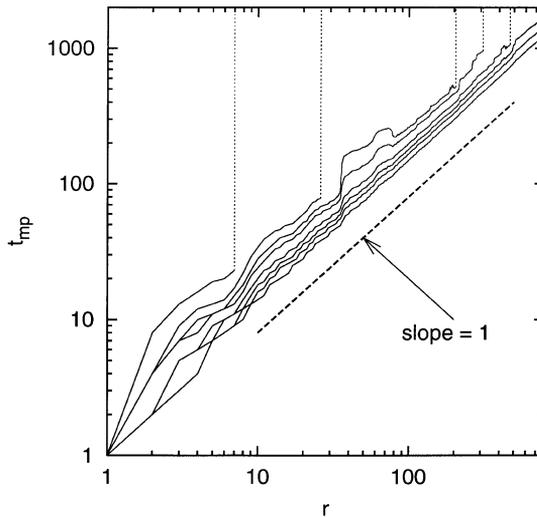


Fig. 4. Most probable path-length as a function of the endpoint separation r , at different temperatures, for a particular realization of disorder. The curves from left to right, are for $T = 1.16, 1.14, 1.12, 1.1, 1.05, 1.01, 0.97, 0.9$. The energies ε_i are in the range $[0.5, 1.5]$. Above a certain temperature T' , which is characteristic of the particular realization of disorder analyzed, the most probable path-length diverges when $r > r^*(T)$ for every $T > T'$, similar to the case of a homogeneous lattice. Unlike homogeneous lattices, the random walk phase is absent.

the temperature T' is *specific to each realization*, and does not characterize the ensemble as a whole.

A general property that describes the full ensemble of disordered lattices is the fraction $f_{\varepsilon,\delta}(T,r)$ of realizations for which the most probable path-length between two points, a distance r apart, diverges at temperature T . In the homogeneous case, $f_{\varepsilon,0}(T,r)$ is the step function:

$$f_{\varepsilon,0}(T,r)|_{r = \text{const.}} = \begin{cases} 0, & T \leq T^*(r), \\ 1, & T > T^*(r). \end{cases} \tag{15}$$

In the presence of disorder, $\delta > 0$, the fraction $f_{\varepsilon,\delta}(T,r)$ obtained numerically has a sigmoid shape. Results for $\varepsilon = 1$ and various values of δ are shown in Fig. 5.

One can see from Fig. 5 that for each range of disorder, $\varepsilon - \delta/2 \leq \varepsilon_i \leq \varepsilon + \delta/2$, there is a temperature $T_{\varepsilon,\delta}^*(r)$ below which $f_{\varepsilon,\delta}(T,r)$ is zero. Consequently, below the asymptotic value $T_c(\varepsilon,\delta) = T_{\varepsilon,\delta}^*(r \rightarrow \infty)$ the quantity $f_{\varepsilon,\delta}(T,r)$ is always zero,

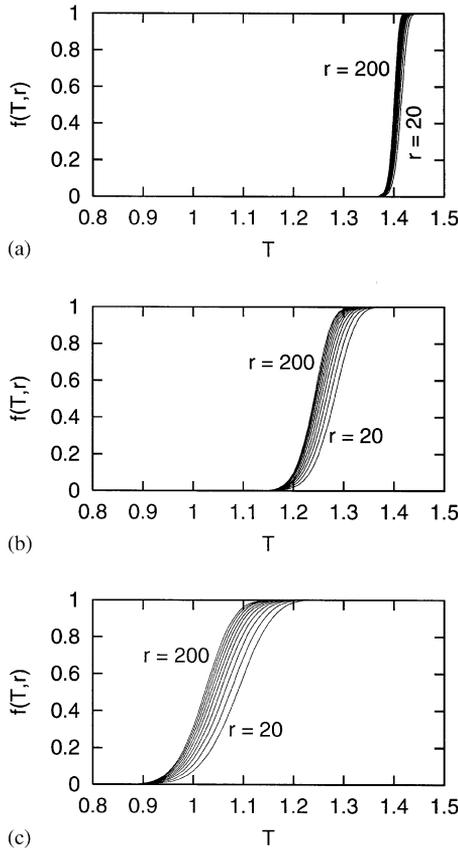


Fig. 5. Fraction of realizations of disorder in which the most probable path-length diverges shown as a function of the temperature T , for disorder range: (a) $0.9 \leq \varepsilon_i \leq 1.1$, (b) $0.7 \leq \varepsilon_i \leq 1.3$, (c) $0.5 \leq \varepsilon_i \leq 1.5$.

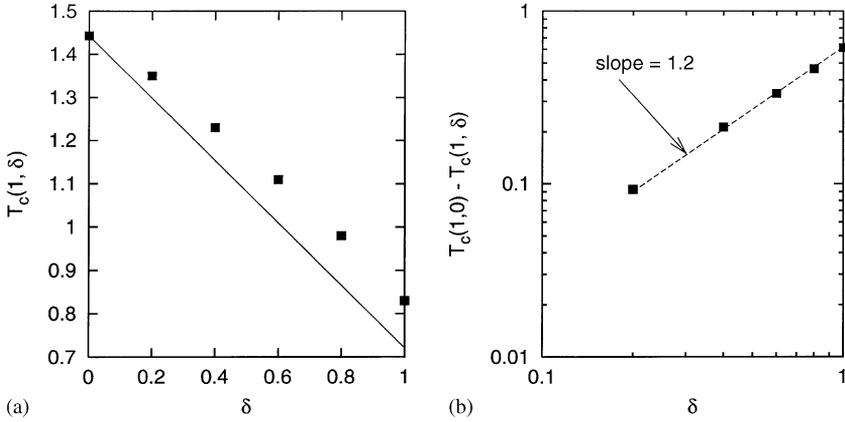


Fig. 6. (a) Critical temperature $T_c(\varepsilon, \delta)$, for $\varepsilon=1$, shown as a function of the width δ of the range of disordered bond energies. The data obtained numerically are found to be above the theoretical lower bound denoted by the solid line. (b) Deviations of the critical temperatures shown in part (a) from that of the homogeneous medium with $\varepsilon=1$ seem to follow a power law.

regardless of the value of r . The temperatures $T_{\varepsilon, \delta}^*(r)$ and $T_c(\varepsilon, \delta)$ are characteristic of the ensemble.

A lower bound for $T_c(\varepsilon, \delta)$ is provided by the extreme case where all the bonds assume the lowest possible energy, $\varepsilon - \delta/2$:

$$T_c(\varepsilon, \delta) \geq T_c\left(\varepsilon - \frac{\delta}{2}, 0\right) = \frac{\varepsilon - \delta/2}{\ln 2} = T_c(\varepsilon, 0) \left[1 - \frac{\delta}{2\varepsilon}\right]. \tag{16}$$

In Fig. 6(a), we show values of $T_c(1, \delta)$ obtained numerically. We also find that $T_c(1, \delta)$ deviates from $T_c(1, 0)$ of the homogeneous system in power-law fashion (Fig. 6b):

$$T_c(1, 0) - T_c(1, \delta) \sim \delta^x, \quad x \approx 1.2. \tag{17}$$

Though our data is for $\varepsilon=1$, we believe that a similar relation holds for other values of $\varepsilon > 0$.

4. Discussion

The central result of this paper is the phase transition in the nature of most probable paths between two fixed points in a one-dimensional lattice with homogeneous bond energy ε . A transition was shown to occur from an optimal-like nature at low temperatures to a random walk form near criticality, and to a discontinuous divergence of the path lengths at temperature $T > T_c = \varepsilon/\ln 2$. The length of the most probable path at any finite temperature is controlled by two opposing factors: the energy of interaction with the lattice and the entropy. At low temperatures ($\varepsilon/T \rightarrow \infty$) the optimal nature of the most probable paths could be attributed to the drive to minimize the energy of

interaction with the lattice, entropy being of negligible consequence. At extremely high temperatures ($\varepsilon/T \rightarrow 0$), the available entropy is large enough for the most probable paths to ignore the interaction with the lattice; consequently the paths assume the form of a random walk and eventually diverge in length.

Remarkably, disorder seems to kill the random walk phase, though the transition to divergent path lengths persists. A likely reason is that the entropy available to the most probable paths is lowered by the pinning of the walks to regions of relatively low energy. It would be interesting to see how our one-dimensional results are modified in higher (spatial) dimensions, where the landscape of disorder is richer due to the possibility of a percolation transition. Also, we offer no explanation for the numerically observed power-law dependence of $T_c(\varepsilon, \delta) - T_c(\varepsilon, 0)$ on δ ; this remains a subject for future research.

Acknowledgements

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