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Energy Barriers for Flux Lines in Three Dimensions

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I determine the scaling behavior of the free energy barriers encountered by a flux line in moving through a three-dimensional random potential. A combination of numerical simulations and analytic arguments suggests that these barriers scale with the length of the line in the same way as the fluctuation in the free energy.

KEY WORDS: Flux lines; random media; energy barriers; glassy systems.

Magnetic flux lines (FL) in high-T_c superconductors are one of the simplest examples of glassy systems.[1,2] In thermal equilibrium, a FL is pinned by defects (oxygen impurities, grain boundaries, etc.) in the superconductor, which lower its energy.[3] This effect is limited by the line tension, which opposes the bending of the line. The resulting free energy landscape for the FL is rather complicated and has many local minima, i.e., metastable states.[4] When an electric current flows through the system, the FL feels a Lorentz force perpendicular to its orientation and to the current direction. As long as the current is not strong enough to overcome the pinning forces, the line moves by thermally activated jumps of line segments between metastable configurations.[5-7] The length of these line segments is estimated by the condition that the free energy barrier for a jump should be of the same order as the gain in free energy due to that jump. These dynamics is believed to be the reason for the nonlinear voltage–current characteristics found in experiments.[3]

Since energy barriers play such an important role in the dynamics of FLs, it is essential to know their properties. The scale of these barriers should grow with observation size L like a power law L^{ψ}. Usually, it is

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assumed that the energy scale in the system is set by the fluctuations in free energy, which increase as L^{θ}, and that therefore $\psi = \theta$.[8,7] However, it is also quite possible that the heights of the ridges in the random energy landscape scale differently from those of the valleys that they separate, with $\psi > \theta$. Yet another scenario is that transport occurs mainly along a percolating channel of exceptionally low energy valleys with $\psi < \theta$. A first attempt to clarify this situation was taken in ref. 9, where $\psi = \theta$ was established for a FL moving in two dimensions. This demonstration relied on exact results for minimal energies in $1+1$ dimensions, and on the fact that the endpoint of a FL in two dimensions has to move through all points which lie between its initial and final positions. It is of great importance to discuss also a FL in three dimensions, which is more physically relevant. In contrast to a two-dimensional system, a FL which moves in three dimensions can avoid regions in space which are energetically unfavorable for one of its segments, and one might therefore speculate that $\psi < \theta$ in three dimensions. In this paper, we first determine numerically a lower bound for the barrier energy which scales in the same way as the energy fluctuations, thus ruling out $\psi < \theta$. Further numerical results predict that an upper bound scales in the same way, ruling out $\psi > \theta$, and thus leading to $\psi = \theta$.

We describe the FL as a directed path in a random medium.[10] The path is discretized to lie on the bonds of a cubic lattice starting at the origin and directed along its (1, 1, 1) diagonal. Each segment of the line can proceed in the positive direction along one of the three axes, leading to a total of 3^t configurations after t steps, with endpoints lying in the plane which is spanned by the points $(t, 0, 0)$, $(0, t, 0)$, and $(0, 0, t)$. A given configuration of the FL is labeled by vectors $\{\mathbf{x}(\tau)\}$ for $\tau = 0, 1, \ldots, t$, giving the transverse coordinates of the FL at each step. The points $\{\mathbf{x}(\tau)\}$ lie on the vertices of a triangular lattice. For a given value of τ, they lie on one of three alternating sublattices.

To each bond on the cubic lattice is assigned a (quenched) random energy equally distributed between 0 and 1. The energy of each configuration is the sum of all random bond energies on the line. For each endpoint $(t, \mathbf{x})$, there is a configuration of minimal energy $E_{\min}(\mathbf{x}|t)$ which can be obtained numerically in a time of order t^3 by a transfer matrix algorithm.[10] The fluctuation in minimal energy is known to scale as $t^{\bar{\theta}}$ with $\bar{\theta} \sim 0.24$, and the transverse fluctuation of the coordinates of minimal paths is known to scale as t^{ζ}, with $\zeta \sim 0.62$.[11] The endpoints of the minimal paths with the lowest energy lie within a distance $\propto t^{\zeta}$ of the origin. Figure 1 shows the minimal energies of paths of length $t = 288$ to endpoints $\mathbf{x}$ with $|\mathbf{x}| < O(t^{\zeta})$. The highest energy in this region is represented in white, the smallest energy in black. The minimal energies are correlated over a distance of the order of t^{ζ}. The distribution of minimal energies is close to a

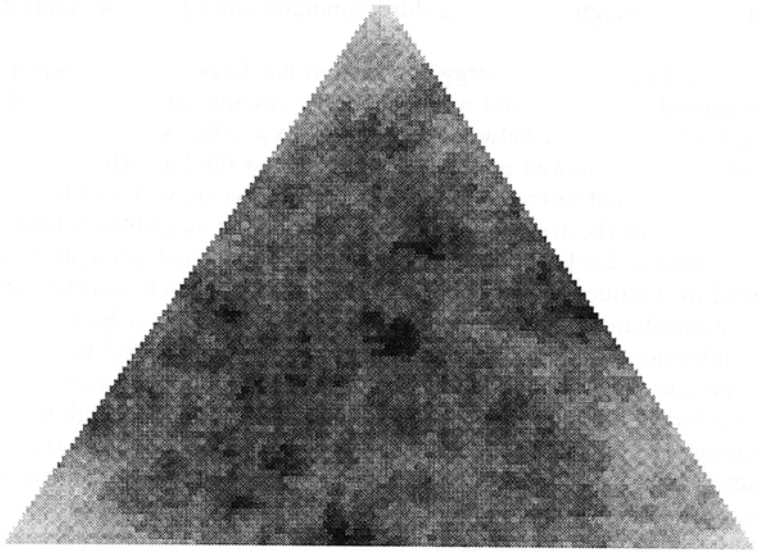

Fig. 1. Minimal energies of paths of length $t = 288$ to endpoints $\mathbf{x}$ with $|\mathbf{x}| < O(t^{\zeta})$. White: High energies; black: low energies.

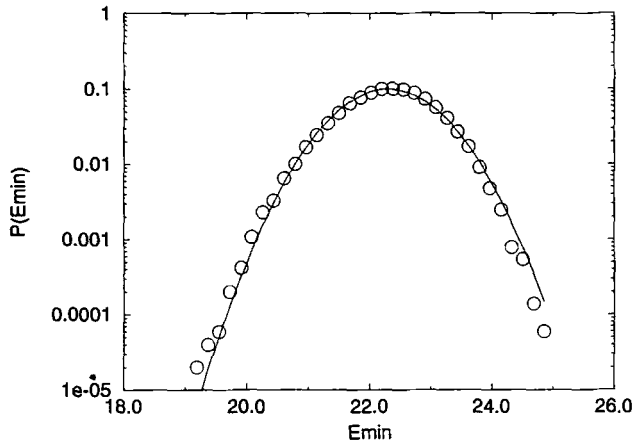

Fig. 2. Probability distribution $P(E_{\min})$ of minimal energies $E_{\min}(\mathbf{0}|144)$, averaged over 50,000 realizations of randomness. The solid line is a Gaussian distribution.

Gaussian and is shown in Fig. 2. Similar to a two-dimensional system,[12] this distribution seems to have a third cumulant since it is not completely symmetric.

We next examine the energy barrier that has to be overcome when the line is moved from an initial minimal energy configuration between $(0, \mathbf{0})$ and $(t, \mathbf{x}_i)$ to a final one between $(0, \mathbf{0})$ and $(t, \mathbf{x}_f)$, with $|\mathbf{x}_{f,i}| \leqslant t^{\zeta}$. The only elementary move allowed is flipping a kink along the line. Thus the point $(\tau, \mathbf{x})$ can be shifted to $(\tau, \mathbf{x} \pm \mathbf{e}_i)$, where $\pm \mathbf{e}_i$ are the six vectors which connect a vertex in the triangular lattice to its nearest neighbors within the same sublattice. Each route from the initial to the final configuration is obtained by a sequence of such elementary moves. For each sequence, there is an intermediate configuration of maximum energy and a barrier which is the difference between this maximum and the initial energy. In a system at temperature T, the probability that the FL chooses a sequence which crosses a barrier of height E_B is proportional to $\exp(-E_B/T)$, multiplied by the number of such sequences. We assume that, as in the case for the equilibrium FL, the "entropic" factor of the number of paths does not modify scaling behavior. Thus at sufficiently low temperatures the FL chooses the optimal sequence which has to overcome the least energy, and the overall barrier is the minimum of barrier energies of all sequences.

Since the number of elementary moves scales roughly as the volume of a cone which contains the initial and final lines, the number of possible sequences grows as $t^{x^2}t$. This exponential growth makes it practically impossible to find the barrier by examining all possible sequences, hampering a systematic examination of barrier energies. Rather than finding the true barrier energy, we proceed by placing lower and upper bounds on it.

A lower bound to the barrier energy is obtained in the following way: While the line moves from its initial to its final configuration, the transverse coordinates of its endpoint move between nearest neighbor positions on one of the above-mentioned triangular sublattices. When the endpoint is at a position $(\mathbf{x})$, the energy of the line is at least as large as the minimal energy $E_{\min}(\mathbf{x}|t)$. The maximum of all these minimal energies along the trajectory of the endpoint, minus the energy of the initial configuration, certainly bounds the barrier energy from below. Since we do not know the actual trajectory of the endpoint, we have to look for the trajectory with the smallest maximal energy. Only in this case can we be sure that we have indeed found a lower bound. This situation is fundamentally different from a two-dimensional system, where there is only one possible trajectory for the endpoint.

Provided that the minimal energies $E_{\min}(\mathbf{x}|t)$ are known, this lower bound is determined in polynomial time by using a transfer-matrix method: We start by assigning to the initial point $\mathbf{x}_i$ a lower bound energy 0, and

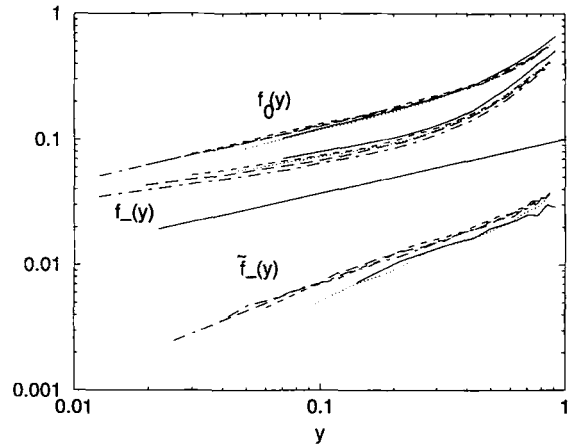

Fig. 3. Scaling functions $f_-(y)$, $\tilde{f}_-(y)$, and $f_0(y)$ defined in Eqs. (1)–(3) for $t=72$ (solid line), $t=144$ (dotted), $t=288$ (dashed), $t=576$ (long-dashed), and $t=1152$ (dot-dashed), averaged over 500 realizations of randomness. The straight line has the slope $\theta/\zeta=0.39$.

to all other sites $\mathbf{x}$ on the same sublattice an energy t which is certainly larger than the lower bound resulting from the algorithm after many iterations. At each step the energy of all sites $\mathbf{x}$ except the initial site is updated according to the following rule: Look for the minimum of the energies of the six neighbors $\mathbf{x}\pm\mathbf{e}_i$. If this is smaller than the energy at $\mathbf{x}$, replace the energy at $\mathbf{x}$ by this minimum or by $E_{\min}(\mathbf{x}\,|\,t)-E_{\min}(\mathbf{x}\,|\,t)$, whichever is larger. After a sufficiently large number of iterations, which is of the order of the size of the area of interest (which scales at $t^{2\zeta}$), all possible trajectories to endpoints within this area have been probed, and the energies no longer change. The energy at site $\mathbf{x}_f$ is then identified as the lower bound. Figure 3 shows the lower bound to the energy barrier for a line with the endpoint moving from the origin to sites within a distance of the order of t^{ζ} for different values of t and averaged over 500 realizations of randomness. The distance $|\mathbf{x}_f-\mathbf{x}_i|$ has been scaled by $t^{-\zeta}$, and the energy by $t^{-\theta}$. With this scaling, all the curves should collapse, leading to the following scaling behavior for the lower bound:

$$\langle E_-(t, |\mathbf{x}_f-\mathbf{x}_i|)\rangle = t^{\theta} f_-(|\mathbf{x}_f-\mathbf{x}_i|/t^{\zeta}) \tag{1}$$

The function $f_-(y)$ is proportional to $y^{\theta/\zeta}$ for small y. For the simulated system sizes, however, this asymptotic scaling cannot yet be clearly seen. For $y>1$, the scaling form in Eq. (1) breaks down since the minimal energy is then a function of the angle $(|\mathbf{x}|/t)$. We conclude that the lower bound to the barrier scales in the same way as the fluctuations in minimal

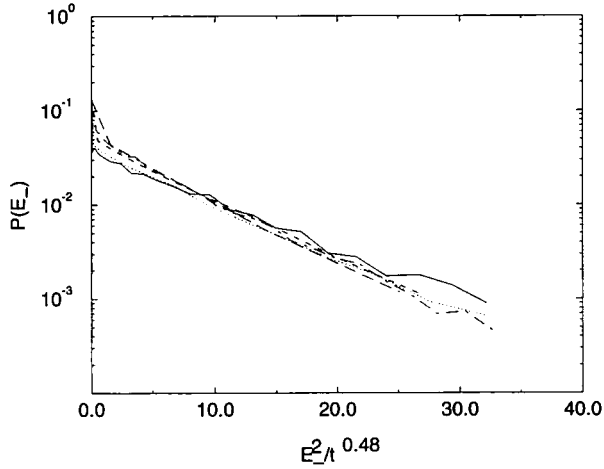

Fig. 4. Probability distribution of E_-. The parameters and symbols are the same as in Fig. 3.

energy, and consequently the energy barrier increases at least as t^θ, leading to $\psi \geqslant \theta$. The distribution $P(E_-)$ of the lower-bound energy for a given distance $|\mathbf{x}| \propto t^\zeta$ is shown in Fig. 4. It appears to be half-Gaussian with width $\propto t^\zeta$.

The result $\psi \geqslant \theta$ is not surprising if one realizes that an even simpler lower bound is given by $\max(E_{\min}(\mathbf{x}_f \mid t) - E_{\min}(\mathbf{x}_i \mid t), 0)$, which evidently scales as t^0 since the distribution function of minimal energies decays exponetially fast, i.e., has no power-law tails (see Fig. 2). To make sure that the scaling of the lower bound found above is not dominated by the neighborhood of final configurations with particularly high energies, I repeated the above simulations by allowing only endpoints with minimal energies smaller than the initial energy. This corresponds to the situation that the endpoint of the line does not move to an arbitrary position, but to a position which is energetically favorable. The result is shown in Fig. 3 and has the scaling form

$$\langle \tilde{E}_-(t, |\mathbf{x}_f - \mathbf{x}_i|) \rangle = t^\theta \tilde{f}_-(|\mathbf{x}_f - \mathbf{x}_i|/t^\zeta) \tag{2}$$

As in the previous case, the asymptotic scaling $\tilde{f}_-(y) \propto y^{\theta/\zeta}$ for small y cannot yet be clearly seen. The energy distribution of the lower bound is again a half-Gaussian of width $\propto t^\zeta$ and looks similar to Fig. 4.

The same scaling behavior is also found when instead of the optimal

trajectory for the endpoint the shortest trajectory (a straight line) is chosen. In this case, the mean of the barrier energy E_0 has the scaling form

$$\langle \tilde{E}_0(t, |\mathbf{x}_f - \mathbf{x}_i|) \rangle = t^{\theta} f_0(|\mathbf{x}_f - \mathbf{x}_i|/t^{\zeta}) \tag{3}$$

(see Fig. 3), again with a half-Gaussian distribution of width $\propto t^{\zeta}$. This, of course, does not represent a lower bound to the true barrier, but it will be important for the determination of an upper bound below, and is therefore included here.

The result $\tilde{E}_- \propto t^{\theta}$ [Eq. (2)] can be explained from the exponential tails of the distribution of minimal energies: If we asume that the endpoint of the line moves only in valleys of particularly low energy, we can successively remove all sites with the largest minimal energy from the set of possible endpoints, until the connectivity over the distance t^{ζ} breaks down. The remaining endpoints form percolation clusters, and their density is given by the corresponding percolation threshold (This is analogous to random resistor networks describing the hopping resistivity for strongly localized electrons. The resistance of the whole sample is governed by the critical resistor that makes the network percolate.[13]) Since the occupied sites are correlated over the distances considered, the value for the threshold is different from the site percolation threshold of 0.5 in an infinite triangular lattice with no correlation between occupied sites. But for the present purpose, it is sufficient to know that this threshold is finite and that therefore a finite percentage of all sites are below threshold. Since the distribution of minimal energies dacays rapidly, its tail cannot contain a finite percentage of all sites. We conclude that the threshold is within a distance of t^{θ} from the peak, and therefore that the energy fluctuation on the percolation cluster and consequently the lower bound for the barrier are $\propto t^{\theta}$.

We now proceed to construct an upper bound to the energy barrier. To this purpose, we specify a sequence of elementary moves which take the line from its initial to its final configuration. Since we cannot be sure that this sequence is the optimal one, we know only that the barrier associated with this specific sequence is an upper bound to the true barrier. The algorithm for the motion of the line is inspired by the one presented in ref. 9 and is as follows: First, one choses a sequence of endpoints connecting the initial to the final endpoint which is as short as possible. Then, one draws all the minimal paths leading to these endpoints. It is certainly advantageous to keep the intermediate paths as close to minimal configurations as possible and therefore to require that the line passes successively through all these intermediate minimal configurations. Usually, minimal configurations $\{\mathbf{x}_1(\tau)\}$ and $\{\mathbf{x}_2(\tau)\}$ with neighboring endpoints have large parts in common and separate only during the last few steps. They enclose a small loop with a size of the order of 1. But sometimes both paths

already separate during the first few steps and form a large loop of the lateral size of the order of t^{ζ}. We have to give a prescription for how the line moves over a loop. If the two minimal paths have nowhere a distance larger than 1 (measured in units of $|\mathbf{e}_i|$), we can choose a sequence of elementary moves such that at most two bonds of the line are not on one or the other minimal path, leading to a barrier of order 1 between the two. If the distance is larger than 1, we proceed as follows: Let τ_0 be the last point which both lines have in common, i.e., $\mathbf{x}_1(\tau_0)=\mathbf{x}_2(\tau_0)$ and $\mathbf{x}_1(\tau_0+1)\neq\mathbf{x}_2(\tau_0+1)$. We then consider the midway points $(\tau_0+(t-\tau_0)/2, \mathbf{x})$ which connect both lines in the middle of the loop via the shortest possible trajectory (if there are several possibilities, we choose one at random). For each of these points, we find two minimal segments of length $(t-\tau_0)/2$ connecting on one side to $(\tau_0, \mathbf{x}_1(\tau_0))$ and on the other to either $(t, \mathbf{x}_1(t))$ or $(t, \mathbf{x}_2(t))$. There are usually several possibilities in making these connections, but all of them lead to the same result. The two segments form an almost minimal path of length $t-\tau_0$, constrained to go through the point $(\tau_0+(t-\tau_0)/2, \mathbf{x})$. We next move the line $\{\mathbf{x}_1(\tau)\}$ with $\tau_0\leqslant\tau\leqslant t$ stepwise through this sequence of almost minimal paths. At each step we first attempt to move the upper segment and then the lower one. The prescription for moving these segments of length $(t-\tau_0)/2$ is exactly the same as for paths of length t: If the distance between two consecutive configurations is larger than 1 for some τ, we consider the points in the middle of the loop formed by the two, and construct minimal paths of half the loop length connecting them to the initial and final loop points. Next we attempt to move segments of the length of the loop by repeatedly moving the upper and lower line portions. In some cases, it is necessary to proceed with this construction until the cutoff scale (1) is reached. Thus, at each intermediate configuration the line is composed of segments of minimal paths of different length, the smallest segments having length 1 in the worst case.

We now estimate the barrier energy resulting from the above construction. In principle, this can be done by programming the algorithm and determining the result numerically. Such a program would be more complicated than in two dimensions, and it would not be able to simulate large systems, since a big portion of the bond energies on the three-dimensional lattice need to be stored. It is therefore uncertain if the asymptotic scaling behavior of the upper bound may be found this way. Instead, we resort to analytic considerations: Since the line is always composed of segments of minimal paths, whose scaling properties are known, we have enough information to give an upper bound to the barrier energy. For small distances $|\mathbf{x}_f-\mathbf{x}_i|$, the initial and final path usually differ only in the last few steps, and therefore the upper bound to the barrier energy (and also the barrier

energy itself) does not depend on t, but only on $|\mathbf{x}_f - \mathbf{x}_i|$. We are interested in the barrier which has to be overcome when the line moves over a distance of the order of t^ζ. Let us add successively the contributions to the upper bound which result from the different steps in the algorithm: The first step consists in finding a sequence of minimal paths with endpoints lying on the shortest trajectory from $\mathbf{x}_i(t)$ to $\mathbf{x}_f(t)$. The energy difference between the minimal path with highest energy and the initial minimal path is $E_0(t, t^\zeta) \sim t^\theta$, which is the first contribution to the upper bound. When moving from one minimal path to the next, the line has to overcome a loop which in the worst case has the length t and which might (again in the worst case) occur in combination with the minimal path with highest energy. We therefore have to add to the upper bound the contribution of a loop of length t and width $\propto t^\zeta$. This is obtained as follows: Within the loop, the line moves through a sequence of paths which are composed of two pieces of minimal path of half the loop length. Both the upper and the lower sequence cover an energy range $E_0(t/2, (t/2)^\zeta) \sim (1/2)^\theta E_0(t, t^\zeta)$. In the worst case, both sequences have their maximum simultaneously, giving a contribution $(1/2)^{\theta-1} E_0(t, t^\zeta)$ to the upper bound. All further contributions can immediately be written down because of the recursive definition of the algorithm: While the upper and lower segments move through minimal configurations within the loop, they in turn have to overcome loops which in the worst case have the size $t/4$, and so on. The sum of all these contributions, averaged over different realizations of randomness, is

$$\begin{aligned} \langle E_c(t, t^\zeta)\rangle &= \langle E_0(t, t^\zeta)\rangle + 2\langle E_0(t, t^\zeta)\rangle[(1/2)^\theta + (1/4)^\theta + \cdots] \\ &= \langle E_0(t, t^\zeta)\rangle[2/(1-(1/2)^\theta) - 1] \simeq 12.0\langle E_0(t, t^\zeta)\rangle \end{aligned} \tag{4}$$

In principle, one has to add a constant which accounts for the breakdown of the scaling form of the energy increase for small loops. But this constant is of the order of one and can be neglected with respect to the terms which increase with t^θ.

There are several configurations of the path which are expected to have the energy E_c. They pass through loops of all sizes and are composed of one minimal segment of length $t/2$, one of length $t/4$, etc., ending with two smallest pieces of length 1. Each of these is a candidate to be the barrier path in our algorithm. To obtain the mean value for the maximum of their energies we need to know their number and their distribution, especially in the large-energy tail. The exact number of candidate barriers is not known, but we can be sure that it increases no faster than $t^{1+\zeta}$ which is the order of the total number of intermediate configurations of the path. The energy distribution for the candidate barriers results from the energy distribution of their segments: Each of the segments of length τ_i has an

approximately (half-)Gaussian energy distribution with a width of the order of τ_i^θ. Since the different segments are constructed through a specific recursive procedure, they might not be independent. If we want to be sure to establish an upper bound, we have to assume the worst case that they are completely dependent, resulting in a variance

$$\begin{aligned} \mathrm{var}(E_c(t, t^\zeta)) &\simeq \log_2(t)[\mathrm{var}(E_0(t, t^\zeta)) + 2\,\mathrm{var}(E_0(t/2, (t, 2)^\zeta)) + \cdots] \\ &\simeq 8.7 \ln(t)\,\mathrm{var}(E_0(t, t^\zeta)) \propto \ln(t)\, t^{2\theta} \end{aligned} \tag{5}$$

It can be checked easily that (for large N), the maximum of N independent Gaussian variables of mean a and variance σ^2, is a Gaussian of mean $a + \sigma(2 \ln N)^{1/2}$ and variance $\sigma^2/(2 \ln N)$. Since the candidate barriers have large segments in common, their energies are not independent. Assuming their independence, we overestimate again the barrier energy, but of course we still establish an upper bound to it. Putting all contributions together and taking into account the behavior for small $|\mathbf{x}_f - \mathbf{x}_i|$, we finally obtain the following estimate for the upper bound in barrier energy:

$$\begin{aligned} \langle E_+(|\mathbf{x}_f - \mathbf{x}_i|, t)\rangle &= \langle E_c(|\mathbf{x}_f - \mathbf{x}_i|, t)\rangle + [2 \ln N\, \mathrm{var}\, E_c(|\mathbf{x}_f - \mathbf{x}_i|, t)]^{1/2} \\ &\simeq (\ln t)\, t^\theta f_+(|\mathbf{x}_f - \mathbf{x}_i|/t^\zeta) \end{aligned} \tag{6}$$

To conclude, I have shown that the energy barrier encountered by a FL moving in a 3D random medium has an upper and a lower bound which both increase with t^θ, except for logarithmic corrections. From this follows that the barrier itself increases with t^θ, confirming the hypothesis $\psi = \theta$. Since the argument presented in this paper is mainly based on the exponential tails of the minimal energy distribution, it can be expected that the result $\psi = \theta$ holds also in higher dimensions, provided that the distribution of minimal energies still has exponential tails.

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