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Variational Approach to Interfaces in Random Media: Negative Variances and Replica Symmetry Breaking

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Abstract. — A Gaussian variational approximation is often used to study interfaces in random media. By considering the 1 + 1 dimensional directed polymer in a random medium, it is shown here that the variational Ansatz typically leads to a negative variance of the free energy. The situation improves by taking into account more and more steps of replica symmetry breaking. For infinite order breaking the variance is zero (*i.e.* subextensive). This situation is reminiscent of the negative entropies in mean field spin glass models, which were also eliminated by considering infinite order replica symmetry breaking.

The subject of interfaces in random media has many applications, such as directed polymers in a random medium, domain walls in dirty magnets, and interfaces in random sponges. Various aspects of this field and methods of approach have been reviewed, see [1-3].

As a tool to get a grip on these complicated objects, a Gaussian variational Ansatz has been proposed by Mézard and Parisi [4] to calculate the free energy. It was found that replica symmetry is broken spontaneously. This variational replica-approach reproduces the Flory values for critical exponents, that can be derived by Flory-Imry-Ma type of estimates.

In the approach an infinity $(k = \infty)$ of replica symmetry breakings occur. Carlucci, de Dominicis and Temesvari have shown that the instability of the replica approach at finite k disappear in the limit $k \to \infty$ [5].

The problem of a directed polymer on a random substrate in d = 1 + 1 has received quite some attention. It was pointed out by Kardar [6] that the replicated free energy can be related to the ground state energy of n interacting bosons in one dimension. This problem can be solved exactly by means of the Bethe Ansatz. The depinning of such a polymer or interface from a wall is also solvable exactly, when the effect of the wall potential is described by a derivative condition of the wavefunction at the wall. Various interesting results have been derived from the exact groundstate wavefunction near the depinning transition [2].

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Here we reconsider the d = 1 + 1 problem of a directed polymer of length L in a random potential. The purpose is not to derive the best variational approximation to the exact solution. Having in mind more complicated models, we wish to test a particular aspect of the variational approach of Mézard and Parisi, that we fully work out for this situation. Due to the one-dimensional character of the problem, we can get the results by studying a quantum Hamiltonian.

In particular we point out that order n^2L terms of the *n*-fold replicated free energy F_n tend to have the wrong sign, so that they tend to predict a negative variance of the physical free energy. This unphysical prediction occurs in case of no replica symmetry breaking and becomes less severe for a finite number of breakings; it seems related to the instability of some fluctuation modes. The whole n^2L term disappears if infinite order replica symmetry breaking is taken into account. The negative variance of the free energy thus plays a role similar to the negative entropy of the SK-model: both vanish only when infinite replica symmetry breaking is taken into account.

The implication of vanishing of the n^2L term is that the fluctuations in the free energy are smaller than $L^{1/2}$ We shall then show that the replicated free energy has leading correction $\sim n^5L$, which means that the free energy fluctuations are of predicted to be of order $L^{1/5}$. This is in agreement with the Flory prediction worked out by Mézard and Parisi. Note that the exact order of magnitude is known to be $L^{1/3}$

In Section 1 we introduce the model and the variational Ansatz. The simplest cases are considered. In Section 2 the problem is solved for infinite order replica symmetry breaking. We close with a summary in Section 3.

1. The Model and the Variational Approach

We consider an interface z(x) with Hamiltonian

$$\beta \mathcal{H} = \int_0^L \mathrm{d}x \left\{ \frac{\gamma}{2} \left(\frac{\mathrm{d}z}{\mathrm{d}x} \right)^2 + V(x, z(x)) \right\}.$$
(1)

 $\beta = 1/T$ is the inverse temperature, $\gamma(T)$ is the interface stiffness, and there is δ -correlated Gaussian disorder

$$\overline{V(x,z)V(x',z')} = \sigma^2 \delta(x-x')\delta(z-z')$$
⁽²⁾

where the overline denotes the average over the quenched disorder. We shall study the partition sum

$$Z = \int \mathrm{D}z \ \mathrm{e}^{-\beta \mathcal{H}} = \mathrm{e}^{-\beta F} \tag{3}$$

(For a formulation on the lattice, see [2].) The replicated partition sum

$$Z_n = \overline{Z^n} \longrightarrow \exp(-\beta F_n) = \overline{\exp(-n\beta F)} = \exp\sum_{k=1}^{\infty} n^k \overline{(-\beta F)_{\rm cum}^k}$$
(4)

generates the cumulants of βF as the expansion coefficients of βF_n for small n. For having a non-negative variance of F the n^2 term of F_n should be non-positive.

Averaging over disorder one obtains the effective n-particle Hamiltonian

$$\mathcal{H}_n = \int_0^L \mathrm{d}x \left\{ \frac{\gamma}{2} \sum_{\alpha=1}^n \left(\frac{\mathrm{d}z_\alpha}{\mathrm{d}x} \right)^2 - \sigma^2 \sum_{\alpha < \beta} \delta(z_\alpha(x) - z_\beta(x)) \right\}.$$
 (5)

By analog with the Feynman-Kac path integral formulation of quantum mechanics, the replicated free energy can be obtained as

$$\beta F_n = L E_n \tag{6}$$

where E_n is the ground state energy of the quantum Hamiltonian

$$H_n = -\frac{1}{2\gamma} \sum_{\alpha=1}^n \frac{\partial^2}{\partial z_{\alpha}^2} - \sigma^2 \sum_{\alpha < \beta} \delta(z_{\alpha} - z_{\beta}).$$
(7)

The expansion

$$E_n = nE^{(1)} + n^2 E^{(2)} + n^3 E^{(3)} + n^4 E^{(4)} + n^5 E^{(5)} + .$$
(8)

determines the cumulants

$$\overline{(\beta F)^k_{\text{cum}}} = (-1)^{k-1} k! L E^{(k)}$$
(9)

The present problem has an exact ground state wavefunction

$$\psi_0(z) = \exp -\kappa \sum_{\alpha < \beta} |z_\alpha - z_\beta| \tag{10}$$

where $\kappa = \sigma^2 \gamma$. The groundstate energy is

$$E_n = \frac{\gamma \sigma^4}{2} \, \frac{n - n^3}{3} \,. \tag{11}$$

To our knowledge, the variational approach to this problem was first formulated by Honeycutt and Thirumalai [7]. They considered a Hartree variational interface Hamiltonian, that we generalize as

$$\mathcal{H}_{n}^{\mathrm{var}} = \int_{0}^{L} \mathrm{d}x \left\{ \frac{\gamma}{2} \sum_{\alpha=1}^{n} \left(\frac{\mathrm{d}z_{\alpha}}{\mathrm{d}x} \right)^{2} - \frac{\gamma}{2} \sum_{\alpha,\beta=1}^{n} z_{\alpha}(q^{2})_{\alpha\beta} z_{\beta} \right\}.$$
 (12)

The original approach had $q_{\alpha\beta} = \delta_{\alpha\beta}q$. The generalized approach is equivalent with the one of Mézard and Parisi, though it is simpler. Indeed, the mapping onto a quantum problem, which can only be done in d = 1 + 1, prevents the introduction of a Fourier wavenumber.

The variational Hamiltonian is equivalent with considering the Hartree variational quantum Hamiltonian

$$H_n^{\text{var}} = -\frac{1}{2\gamma} \sum_{\alpha=1}^n \frac{\partial^2}{\partial z_\alpha^2} - \frac{\gamma}{2} \sum_{\alpha,\beta=1}^n z_\alpha (q^2)_{\alpha\beta} z_\beta$$
(13)

which has the groundstate wavefunction

$$\psi(\{z_{\alpha}\}) = \frac{1}{(\det \pi q)^{1/4}} e^{-\frac{1}{2} \sum_{\alpha,\beta=1}^{n} z_{\alpha} q_{\alpha\beta} z_{\beta}}$$
(14)

The ground state energy now is approximated as

$$E_n = E_n^{\text{var}} + \langle \psi | (H_n - H_n^{\text{var}}) | \psi \rangle.$$
(15)

Rescaling $q \to 2\sigma^4 \gamma^2/\pi$ we have

$$E_n = \frac{\gamma \sigma^4}{2\pi} \tilde{E}_n \tag{16}$$

with

$$\tilde{E}_n = \sum_{\alpha} q_{\alpha\alpha} - \sum_{\alpha \neq \beta} \frac{2\sqrt{2}}{\sqrt{(q^{-1})_{\alpha\alpha} + (q^{-1})_{\beta\beta} - 2(q^{-1})_{\alpha\beta}}}.$$
(17)

The exact value would correspond to $\tilde{E}_n = \pi (n - n^3)/3$. We shall now consider various choices for the shape of $q_{\alpha\beta}$.

1.1. DIAGONAL q. — The case $q_{\alpha\beta} = q_d \delta_{\alpha,\beta}$ was studied by Honeycutt and Thirumalai. Optimizing E_n yields $q_d = (n-1)^2$, so that

$$\tilde{E}_n = -n(n-1)^2 \tag{18}$$

which differs in sign from the Honeycutt-Thirumalai result. Since our n^2 term is positive, we conclude that this result leads to a negative variance of F, and is not acceptable.

1.2. TRANSLATIONAL INVARIANCE AND OFF-DIAGONAL q

1.2.1. Replica symmetry. — If there is no RSB then we can set $q_{\alpha\beta} = (q_d - q_0)\delta_{\alpha,\beta} + q_0$.

$$\tilde{E}_n = nq_d - 2n(n-1)\sqrt{q_d - q_0}.$$
(19)

The structure of this expression shows that we only get a well posed problem if we relate q_0 and q_d in some way. Above we considered $q_0 = 0$ but the result was unsatisfactory. As we have averaged over disorder, there is translational invariance. One would expect that the physically relevant variational Ansatz reflects the translational invariance of the replicated problem. Hereto we have to impose

$$\sum_{\beta} q_{\alpha\beta} = 0. \tag{20}$$

This condition is equivalent to staying in the "replicon' or "ergodon" subspace. implying here that $q_d + (n-1)q_0 = 0$. This allows to eliminate q_d , after which we get

$$\dot{E}_n = -n(n-1)q_0 - 2n(n-1)\sqrt{-nq_0}.$$
(21)

The saddle point is $q_0 = -n$, yielding

$$\tilde{E}_n = -n^2(n-1).$$
 (22)

This result has $E_0 = 0$ and variance -1, in both respects better than previous case. But also this result leads to a negative variance, and is not acceptable.

1.2.2. One Step Replica Symmetry Breaking. — Now we choose

$$q_{\alpha\beta} = (q_d - q_1)\delta_{\alpha\beta} + (q_1 - q_0)\mathcal{E}^{(x_1)}_{\alpha\beta} + q_0\mathcal{E}^{(n)}_{\alpha\beta}$$
(23)

where $\mathcal{E}^{(x_1)}$ is the Parisi 1RSB matrix having n/x_1 diagonal $x_1 \times x_1$ blocks with elements equal to unity. (Thus $\mathcal{E}^{(1)}$ is the identity matrix, while $\mathcal{E}^{(n)}$ is a matrix with all elements equal to unity.) Due to translational invariance we may eliminate q_d and get

$$q_d = -(x_1 - 1)q_1 - (n - x_1)q_0.$$
⁽²⁴⁾

The inverse reads

$$q_{\alpha\beta}^{-1} = \frac{\delta_{\alpha\beta}}{q_d - q_1} - \frac{q_1 - q_0}{(q_d - q_1)(q_d - (1 - x_1)q_1 - x_1q_0)} \mathcal{E}_{\alpha\beta}^{(x_1)} - \frac{q_0}{(q_d - (1 - x_1)q_1 - x_1q_0)(q_d - (1 - x_1)q_1 - x_1q_0 + nq_0)} \mathcal{E}_{\alpha\beta}^{(n)}.$$
(25)

The last factor diverges in case of translational invariance. Fortunately, it generally cancels from our expression for \tilde{E}_n . We thus obtain

$$\tilde{E}_{n} = n(1-x_{1})q_{1} + n(x_{1}-n)q_{0} + 2n(1-x_{1})\sqrt{-x_{1}q_{1} + (x_{1}-n)q_{0}} + 2n(x_{1}-n)\sqrt{\frac{(-x_{1}q_{1} + (x_{1}-n)q_{0})(-nq_{0})}{-q_{1} + (1-n)q_{0}}}.$$
(26)

This has the same $\sqrt{-nq_0}$ behavior as above. Setting

$$q_0 = -nr \tag{27}$$

we get up to order n^2

$$\tilde{E}_n = n(1-x_1)q_1 - n^2 x_1 r + 2n(1-x_1)\sqrt{-x_1q_1} - n^2 \frac{x_1(1-x_1)}{\sqrt{-x_1q_1}r} + 2n^2 x_1 \sqrt{x_1 r}.$$
(28)

Optimization yields $q_1 = -x_1 + \mathcal{O}(n)$, so

$$\tilde{E}_n = nx_1(1-x_1) - n^2r + 2n^2x_1\sqrt{x_1r}.$$
(29)

Further optimization fixes $x_1 = 1/2$, $r = x_1^3 = 1/8$, which finally yields

$$\tilde{E}_n = \frac{1}{4}n + \frac{1}{8}n^2.$$
(30)

The n^2 term is smaller than without replica symmetry breaking but still of wrong sign. We must allow for more breakings.

2. Infinite Order Replica Symmetry Breaking

Now let us extend the above approach and consider k-step RSB. Let us consider the following representation for a matrix q:

$$q_{\alpha\beta} = (q_d - q_k)\delta_{\alpha\beta} + \sum_{i=0}^k (q_i - q_{i-1})\mathcal{E}_{\alpha\beta}^{(x_i)}$$
(31)

where $q_{-1} \equiv 0$, $x_j < x_{j-1}$ and $x_{k+1} = 1$, $x_0 = n$. It thus holds $\mathcal{E}^{(x_k)}\mathcal{E}^{(x_k)} = x_j\mathcal{E}^{(x_k)}$ when $x_j < x_k$. The eigenvalues of $q_{\alpha\beta}$ are

$$\lambda_{k} = q_{d} - q_{k}$$

$$\lambda_{i} = q_{d} - x_{i+1}q_{i} - \sum_{j=i+1}^{k} (x_{j+1} - x_{j})q_{j} \qquad i = 0, \cdot ..., k - 1$$

$$\lambda_{-1} = nq_{0} + \lambda_{0}.$$
(32)

Translational invariance implies $\lambda_{-1} = 0$. Expressing q in the λ 's we get

$$q_{\alpha\beta} = \lambda_k \delta_{\alpha\beta} + \sum_{i=0}^k \frac{\lambda_{i-1} - \lambda_i}{x_i} \mathcal{E}_{\alpha\beta}^{(x_i)}.$$
(33)

Its inverse has the same structure, so it can be written

$$q_{\alpha\beta}^{-1} \equiv b_{\alpha\beta} = (b_d - b_k)\delta_{\alpha\beta} + \sum_{i=0}^k (b_i - b_{i-1})\mathcal{E}_{\alpha\beta}^{(x_i)}$$
$$= \frac{1}{\lambda_k} + \sum_{i=0}^k \frac{1/\lambda_{i-1} - 1/\lambda_i}{x_i}\mathcal{E}^{(x_i)}$$
(34)

Let us define

$$r_{\alpha\beta} = (q^{-1})_{\alpha\alpha} - (q^{-1})_{\alpha\beta}.$$
(35)

It has elements r_i

$$r_{i} = \frac{1}{\lambda_{k}} + \sum_{j=i+1}^{k} \frac{1}{x_{j}} \left(\frac{1}{\lambda_{j-1}} - \frac{1}{\lambda_{j}} \right).$$
(36)

The replicated energy becomes

$$\frac{\tilde{E}_n}{n} = (x_1 - n)q_0 + \sum_{i=1}^k (x_{j+1} - x_i)q_i + 2\frac{x_0 - n}{\sqrt{r_0}} + 2\sum_{i=1}^k \frac{x_{i+1} - x_i}{\sqrt{r_i}}$$
(37)

where $x_{k+1} \equiv 1$. This can be rewritten as

$$\tilde{E}_n = n\tilde{E}^{(1)} + n^2 \Delta_n \tag{38}$$

with

$$\tilde{E}^{(1)} = \sum_{i=1}^{k} \left\{ \left(\frac{1}{x_{i+1}} - \frac{1}{x_i} \right) \lambda_i + \frac{2(x_{i+1} - x_i)}{\sqrt{r_i}} \right\}$$
(39)

and

$$\Delta_n = \left(\frac{1}{x_1} - \frac{1}{n}\right) \frac{\lambda_0}{n} + \frac{2(x_1 - n)}{n\sqrt{r_0}}.$$
(40)

Only the terms in Δ_n depend explicitly on n. Using $r_0 = r_1 + (1/\lambda_0 - 1/\lambda_1)/x_1$, which follows from (36), the dependence on λ_0 has been made explicit. The saddle point w.r.t. λ_0 yields

$$\lambda_0 = \frac{n^2 x_1^3}{(1 + \lambda_0 (x_1 r_1 - \frac{1}{\lambda_1}))^3} \approx n^2 x_1^3 (1 - 3n^2 x_1^3 (x_1 r_1 - \frac{1}{\lambda_1})) + \cdot$$
(41)

in agreement with previous finding $\lambda_0 = -nq_0 \sim +n^2$. We can now expand Δ_n in powers of n

$$\Delta_n = x_1^3 - nx_1^2 - n^2 x_1^6 (x_1 r_1 - \frac{1}{\lambda_1}) + n^3 x_1^5 (x_1 r_1 - \frac{1}{\lambda_1}) + \cdot$$
(42)

With this form for Δ_n , \tilde{E}_n has to be optimized in x_1, \dots, x_k and $\lambda_1, \dots, \lambda_k$. The n^2 term of \tilde{E}_n has prefactor x_1^3 , which is expected to vanish for $k \to \infty$. So infinite replica symmetry breaking cures the problem of negative variances. We have thus reached the main point of this work. It remains to be shown that the leading term (which is of order n^5), has a non-vanishing prefactor. Before doing that we calculate the average free energy.

2.1. THE AVERAGE FREE ENERGY. — Let us now calculate the $\mathcal{O}(n)$ value of \tilde{E}_n and later the leading correction, that will turn out to be of order n^5 . In the continuum limit one gets from equation (37)

$$\tilde{E}^{(1)} = \int_0^1 \mathrm{d}x \ q(x) + 2 \int_0^1 \frac{\mathrm{d}x}{\sqrt{r(x)}}$$
(43)

$$r(x) = \frac{x}{\lambda(x)} - \int_{x}^{1} \frac{\mathrm{d}y}{y^{2}\lambda(y)} \longrightarrow r'(x) = \frac{q'(x)}{\lambda^{2}(x)}$$
(44)

$$\lambda(x) = -xq(x) + \int_0^x \mathrm{d}y \ q(y) \longrightarrow \lambda'(x) = -xq'(x). \tag{45}$$

We search a solution non-constant q(x) for $0 < x < \bar{x}$, while $q(x) = \bar{q}$ for $\bar{x} < x < 1$ for some \bar{x} . Variation with respect to q(z) yields

$$\frac{1}{r^{3/2}(z)\lambda^2(z)} - \int_z^{\bar{x}} \frac{\mathrm{d}x}{xr^{3/2}(x)\lambda^2(x)} - \frac{1}{z\lambda(z)^2} \int_0^z \frac{\mathrm{d}x}{r^{3/2}(x)} + \int_z^{\bar{x}} \frac{\mathrm{d}y}{y^2\lambda^2(y)\int_0^y \frac{\mathrm{d}x}{r^{3/2}(x)}} = 1.$$
(46)

Differentiation with respect to z yields q'(z) = 0 or

$$-\frac{1}{r^{5/2}(z)\lambda(z)} + \frac{2z}{r^{3/2}(z)} - 2\int_0^z \frac{\mathrm{d}x}{r^{3/2}(x)} = 0.$$
(47)

Taking two more derivatives one obtains

$$r(z)\lambda(z) = \frac{5}{6z}.$$
(48)

Inserting this in equation (47) one gets an equation for r alone. This yields

$$r(x) = \frac{A}{x^6} \longrightarrow \lambda(x) = \frac{5x^5}{6A}$$
(49)

with some A. Inserting this in equation (44) one finds

$$\bar{x} = \frac{5}{6} \tag{50}$$

and finally from (46) one obtains

$$q(x) = -\frac{23^9 x^4}{\frac{5^6}{5^8}}$$
(51)

$$r(x) = \frac{5^{6}}{2^{4}3^{10}x^{6}}$$
(52)

$$\Lambda(x) = \frac{2^{5}3^{5}x^{5}}{5^{7}}.$$
 (53)

The average free energy is determined by

$$\tilde{E}^{(1)} = \int_0^{\bar{x}} q(x) dx + (1 - \bar{x}) \tilde{q} + 2 \int_0^{\bar{x}} \frac{dx}{\sqrt{r(x)}} + 2 \frac{1 - \bar{x}}{\sqrt{\bar{r}}} = \frac{27}{100}.$$
(54)

This value is approximately 4 times smaller than the exact value $\pi/3$.

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2.2. CUMULANTS OF THE FREE ENERGY. — Next we consider the higher powers in n, coded in equation (42) for Δ_n . For our purpose we may calculate it using the n = 0 expressions for the x_i and λ_i . The terms of order n^0 , n^1 and n^2 have too many powers of x_1 and vanish for $k \to \infty$, where $x_1 \to 0$. The n^3 term yields

$$\tilde{E}^{(5)} = x_1^6 r_1 - \frac{x_1^5}{\lambda_1}.$$
(55)

Using the continuum results (51) it can be estimated by setting $r_1 \approx r(x_1)$, $\lambda_1 \approx \lambda(x_1)$

$$\tilde{E}^{(5)} \approx -\frac{5^7}{2^4 3^{10}}.$$
(56)

The correct approach is to calculate r_1 and λ_1 at finite but large k. At n = 0 this can be done quite simply. Taking derivatives of (39) with respect to λ_1 and x_1 we obtain,

$$\frac{1}{x_2} - \frac{1}{x_1} - \frac{x_2 - x_1}{r_1^{3/2}} \frac{-1}{x_2 \lambda_1^2} = \frac{\lambda_1}{x_1^2} - \frac{2}{\sqrt{r_1}} = 0,$$
(57)

respectively. x_2 can be eliminated, and we get

$$\lambda_1 = 8x_1^5 \qquad r_1 = \frac{1}{16x_1^6}$$
 (58)

We do not need the value of x_1 here, and obtain immediately

$$\tilde{E}^{(5)} = x_1^6 r_1 - \frac{x_1^5}{\lambda_1} = -\frac{1}{16}.$$
(59)

The prefactor in the estimate (56) has the same sign but is larger by a factor 1.32305. This result thus proves the leading behavior

$$\overline{(-\beta F)^5_{\rm cum}} = \frac{5!}{16} L \frac{\gamma \sigma^4}{2\pi} \tag{60}$$

which has the expected sign. In other words, in the variational approach free energy fluctuations are predicted to be of order $L^{1/5}$

3. Summary

In the present work we have extended the variational approach of Honeycutt and Thirumalai to directed polymers in 1 + 1 dimensional random media. This is a toy model for the more general field of interfaces in random media, considered by Mézard and Parisi. In our problem a mapping on a Schrödinger equation is possible, which prevents the need of space-dependent propagators and the occurrence of wavenumbers.

We have reconsidered the variational Ansatz of Honeycutt and Thirumalai. We have shown that it leads to a negative variance of the physical free energy, and thus is not a correct Ansatz.

Next we have extended this Ansatz by allowing off-diagonal components of the matrix $q_{\alpha\beta}$. It was observed that an extra constraint is needed to make the problem well posed. The only natural and realistic candidate is spatial translational invariance of the variational wavefunction in replica space. In doing so, we have seen that both the replica symmetric and one-step replica symmetry broken solutions still lead to a negative variance, though it has become smaller. We observe that more and more breakings improves the matter and that for infinite breaking the variance of the free energy has become zero (to leading order in the system size L). Infinite order breaking was also assumed by Mézard and Parisi. We find that the first non-vanishing cumulant is the fifth one, implying free energy fluctuations of order L^{χ} with $\chi = 1/5$, which agrees with the estimate of Mézard and Parisi. Let us recall that this is the Flory or mean field estimate; loop effects should modify it to yield the exact result $\chi = 1/3$.

This present situation of negative variances is reminiscent of the mean field model of spin glasses, SK-model, where an infinity of breaking was needed to obtain a vanishing zero-point entropy. Both effects are related with disappearance of unstable modes in the limit of infinite breaking.

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