Statistical mechanics of strings on periodic lattices

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We present a simple model for string statistics on a periodic lattice. We show how the fraction of topological (infinite) string depends on lattice size and compare our results to those of established numerical simulations.

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In recent years there have been several large-scale numerical simulations [1–6] of string formation. For simplicity, these simulations were performed on periodic lattices. Those of [3–5], in particular, paid considerable attention to the existence of a new phase of long string that was a direct consequence of the periodic boundaries. We shall provide a simple interpretation of this phase and show how it, and several other aspects of the numerical simulations, can be derived analytically in a simple model of string formation. In this model, in which strings are assumed to behave as random walks, it is possible to assess the influence of finite system size on the predictions for string distributions. This is important in that finite size (with periodic boundaries) was always an artifact of the calculational scheme, and not a reflection of the physics.

Our primary motivation for investigating string formation stems from the possibility that a network of cosmic strings, left over from an early grand unified theory phase transition, could provide an explanation for the observed large-scale structure in the Universe [7–9]. Strings themselves occur in many branches of physics, from polymer structures and topological defects in liquid crystals [10,11] to the observation of vortices in the λ transition of ^{4}He and type II superconductors [12]. All this serves as further motivation for our work.

For the purpose of the model we perform all our calculations in thermal equilibrium at a temperature T_s in a periodic box of side d. As we shall see, the critical temperature is defined to be that temperature at which the free energy $E-TS$ vanishes. It is the Hagedorn temperature, above which the canonical partition function for the strings diverge [16]. It turns out for cosmic strings that T_s is closely related to the usual Ginsburg temperature [18], defined as the temperature at which thermal fluctuations in the scalar field become small enough that the domain structure of the phase transition is established. Thus we see that $T_s < T_c$ where T_c is the critical temperature above which the full unbroken symmetry is restored.

For simplicity we assume that the energy of a string is proportional to its length L ($E = \sigma L$) and that the strings are both noninteracting and static. This latter assumption may seem unreasonable for cosmic strings. However, the underlying quantum mechanics of such strings enables us to trade dynamical degrees of freedom for temperature-dependent string parameters in static strings [15]. Moreover, interactions and rigidity can be incorporated, but they only lead to inessential complications.

Numerical results have shown that at the phase transition, to a good approximation, strings can be thought of as classical Brownian random walks [1,13]. Were strings infinitely thin they would have an infinite number of degrees of freedom, since they could bend on any scale. In order to evaluate $\Omega(E,V)$, the density of string states in a periodic volume V (i.e., a torus), we must impose a lower cutoff a on the scale on which the strings can bend, corresponding to the fundamental lattice spacing we adopt. For quantum strings we can either relate the cutoff to the string tension [14], if we take them to be fundamental (i.e., infinitely thin), or identify it with the relevant effective Compton wavelength if the strings are to be considered as hot vortices (see [15], for example). The Compton wavelength at formation is, in fact, the initial correlation length of the scalar field, $\xi(T_s) \equiv m_\phi^{-1}(T_s)$ where m_ϕ is the temperature-dependent mass of the scalar field. Hence we see that the lower cutoff scale a is determined by $\xi(T_s)$.

Furthermore, to simplify computation, we will restrict the strings to lie on a cubic lattice of coordination number $\lambda = 6$ [17]. If backtracking of the string is not forbidden the procedure will give rise to some overcounting. However, the effect will be seen to be very small at the critical temperature and we shall let it stand, except in that the smallest loop will have four segments joining vertices (links). Finally, all our strings are closed. Closure is crucial for the long string phase and for the numerical simulations whose behavior we are trying to derive analytically.

The number of configurations of an open string of length L is $\lambda^{L/a}$ (i.e., entropy $S = (L\ln\lambda)/a$) and thus for closed strings

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$$\Omega(E,V) = \lambda^{L/a} P(L,V), \tag{1}$$

where $P(L,V)$ is the sum of probabilities over all lattice sites that a string of length L will close. Using this expression implies that the partition function for a single string is of the form

$$Z^1 = \sum_L P(L,V) e^{-\beta\sigma_{\rm eff} L}, \tag{2}$$

where $\beta \equiv T^{-1}$, σ is the string tension, $\sigma_{\rm eff}$ the effective string tension,

$$\sigma_{\rm eff} = (E - TS)/L = \sigma\,(1 - T/T_s)\,, \tag{3}$$

and T_s is the Hagedorn temperature, defined by $T_s = \sigma a/\ln\lambda$. The partition function for an ensemble of strings is (in the absence of interactions) $Z = \exp(Z^1)$. Above the Hagedorn temperature the effective string tension is negative and the canonical partition function diverges exponentially [16].

Cosmic strings are composite (i.e., they are composed of more fundamental scalar and gauge fields), unlike the case of fundamental strings [14]. For composite strings the consequences of increasing the temperature above T_s towards T_c where the full symmetry of the theory is restored are dramatic. The effective width of the defects become so large they essentially overlap leading to indistinguishable objects. Hence the concept of a string configuration becomes ill defined as the fundamental fields remain, but no longer in the string configuration. Thus the Hagedorn temperature marks the period in the thermal transition below which strings exist as well-defined objects.

In order to calculate $P(L,V)$, let $p(\mathbf{r}',\mathbf{r},L/a)$ denote the probability density that a string of $L/a = n$ steps begins at $\mathbf{r}'$ and ends at $\mathbf{r}$. In the limit $n\to\infty$, $a\to 0$, and $La = $ const, $p(\mathbf{r}',\mathbf{r},L/a)$ satisfies the heat equation (setting $\lambda = 6$) [17]

$$\frac{\partial p}{\partial n} = \frac{a^2}{6}\nabla^2 p. \tag{4}$$

We can incorporate more physics into the model by adding correction terms proportional to p to the right-hand side of (4). For example, excluded volumes can be modeled using a term $h(\mathbf{r})p$, where $h(\mathbf{r})$ denotes the fraction of space from which the end points of the string segments are excluded [17]. However, although excluded volume has to be taken into account, we shall simulate it more simply (at the end of this paper) by the introduction of a parameter κ describing the maximum allowed fraction of space which can be filled with string. Hence we persist with (4). The solution to the uncorrected equation is the heat-kernel expansion

$$\begin{aligned} p(\mathbf{r}',\mathbf{r},L/a) &\equiv p(\mathbf{r}'-\mathbf{r};L/a) \\ &= \sum_k f_k(\mathbf{r}') f_k^*(\mathbf{r}) e^{-E_k L/a}, \end{aligned} \tag{5}$$

where $f_k(\mathrm{r})$ are the normalized eigenfunctions of

$$-\frac{a^2}{6}\nabla^2 f_k = E_k f_k \tag{6}$$

and the constraints on k are governed by the boundary conditions of the system, as we shall shortly see. Since we are assuming that all strings are closed, $P(L,V)$ is given by the sum over all lattice sites of the probabilities of first return $p(\mathbf{r},\mathbf{r},L/a) = p(\mathbf{0};L/a)$

Using the normalization condition

$$\sum_{\mathbf{r}} |f_k(\mathbf{r})|^2 = 1 \tag{7}$$

we obtain the single-loop partition function

$$Z^1_{\rm loop} = \sum_L \frac{a}{L}\sum_{\mathbf{r}} p(\mathbf{0};L/a) e^{-\beta\sigma_{\rm eff}L} \tag{8}$$

$$= \sum_L \frac{a}{L}\sum_k e^{-E_k L/a - \beta\sigma_{\rm eff}L} \tag{9}$$

$$= \sum_L N(L,\beta), \tag{10}$$

where the factor a/L removes the overcounting due to the degeneracy of the starting positions on the loops and $N(L,\beta)$ is the loop distribution function at $T = \beta^{-1}$. The partition function counts the number of loops of all lengths. Therefore, at the phase transition when $\sigma_{\rm eff} = 0$ the loop distribution function is

$$N(L) = \frac{a}{L}\sum_k e^{-E_k L/a}, \tag{11}$$

we have dropped the β dependence to signify that we are working at the critical temperature, at which the effective energy cost for producing string is zero.

In the numerical simulations it is $N(L)$ that is studied most carefully. They consist of throwing down random field phases on the lattice, and then identifying the vortices that arise. As such, there is no direct identification with the form (11). The simplification comes after establishing the random nature of the strings produced in this process [1,13], allowing $N(L)$ to be calculable analytically.

We begin our analysis by considering a system with infinite volume. The normalized eigenfunctions of equation (6) are of the form

$$f_k(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad E_k = \frac{a^2\mathbf{k}^2}{6}, \tag{12}$$

where $|\mathbf{k}|$ takes the values $0 \le |\mathbf{k}| < \infty$. Substituting into Eq. (5) and writing the sums as integrals we find

$$p(\mathbf{r}'-\mathbf{r};L/a) = \frac{a^3}{(2\pi)^3}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r}) - aL\mathbf{k}^2/6}. \tag{13}$$

Completing the square and integrating over $\mathbf{k}$ reproduces the well-known Gaussian probability distribution

$$p(\mathbf{r}'-\mathbf{r};L/a) = \left(\frac{3a}{2\pi L}\right)^{3/2} e^{-3(\mathbf{r}'-\mathbf{r})^2/2aL}. \tag{14}$$

This expression ought to include a coefficient $\theta(L - |\mathbf{r}'-\mathbf{r}|)$ to ensure that no string can have an extension greater than its length. However, the Gaussian factor damps the probability sufficiently to accommodate this.

If we consider a subvolume d^3, substituting our expression for $p(\mathbf{r};L/a)$ into Eq. (8) and integrating over the volume we find that the loop distribution function for an infinite lattice is

$$N(L) = \frac{a}{L}\int_{d^3} d^3\mathbf{r}\frac{a^3}{(2\pi)^3}\int d^3\mathbf{k}\, e^{-aL\mathbf{k}^2/6} \tag{15}$$

$$= \frac{d^3}{a^2L}\left(\frac{3a}{2\pi L}\right)^{3/2}, \tag{16}$$

which reproduces the $L^{-5/2}$ dependence observed in all the simulations [1–6].

Defining the string density to mean the fraction of links covered by string, the corresponding density of string for an infinite system is

$$\Lambda_\infty = \lim_{d\to\infty}\left(\frac{a}{d}\right)^3\sum_4^\infty LN(L) = \left(\frac{3}{2\pi}\right)^{3/2}. \tag{17}$$

This result is in agreement with the work of [13] in which strings are formed on an infinite lattice but can be either opened or closed. In our formalism open strings are not accounted for, although it is clear that if (as in [13]) all the links of the lattice were filled with string, then a fraction $1-\Lambda_\infty = 0.67$ of the links would be from infinite string.

Having established how strings should form in systems with infinite boundaries, we now turn our attention to the effect of imposing periodic boundaries. For a periodic box of side d the normalized eigenfunctions of Eq. (6) are given by

$$f_k(\mathbf{r}) = \left(\frac{a}{d}\right)^{3/2} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \mathbf{k} = \frac{2\pi}{d}\mathbf{u}, \tag{18}$$

where $\mathbf{u} = (l,m,n)$ and l, m, and n take all integer values, with corresponding eigenvalues

$$E_k = \frac{2\pi^2u^2a^2}{3d^2}. \tag{19}$$

Using these results gives the probability distribution

$$p(\mathbf{r}'-\mathbf{r};L/a) = \left(\frac{a}{d}\right)^3 \vartheta_3\left(\frac{\pi(x'-x)}{d}\,\middle|\,\frac{2\pi iaL}{3d^2}\right) \times\vartheta_3\left(\frac{\pi(y'-y)}{d}\,\middle|\,\frac{2\pi iaL}{3d^2}\right) \times\vartheta_3\left(\frac{\pi(z'-z)}{d}\,\middle|\,\frac{2\pi iaL}{3d^2}\right), \tag{20}$$

where ϑ_3 is the Jacobi theta function. Summing over all lattice sites, the loop distribution function is

$$N(L) = \frac{a}{L}\vartheta_3^3\left(0\,\middle|\,\frac{2\pi iaL}{3d^2}\right), \tag{21}$$

or equivalently

$$N(L) = \frac{d^3}{a^2L}\left(\frac{3a}{2\pi L}\right)^{3/2}\vartheta_3^3\left(0\,\middle|\,\frac{3id^2}{2\pi aL}\right) \tag{22}$$

$$= \frac{d^3}{a^2L}\left(\frac{3a}{2\pi L}\right)^{3/2}\sum_{l',m',n'} e^{-2\pi^2aL(l'^2+m'^2+n'^2)/3d^2} \tag{23}$$

after inversion. By inverting the theta functions we, in effect, introduce a winding vector $\mathbf{u}' = (l',m',n')$, where l', m', and n' are the winding numbers around the three axes, i.e., we can decompose $N(L)$ in an obvious way as

$$N(L) = \sum_{\mathbf{u}'} n_{\mathbf{u}'} = \sum_{l',m',n'} n_{l'm'n'}. \tag{24}$$

Consider now the behavior of the loop distribution function in the large and small loop regimes. Since $\lim_{x\to\infty}\vartheta_3(0|x) = 1$, taking the short-loop limit $L \ll d^2/a$ in Eq. (22) gives

$$N(L \ll d^2/a) \simeq \frac{d^3}{a^2L}\left(\frac{3a}{2\pi L}\right)^{3/2}\left(1 + 6e^{-3d^2/2aL} + \cdots\right). \tag{25}$$

Neglecting exponentially small factors reproduces the expected $L^{-5/2}$ behavior for Brownian strings in an infinite system [1,18].

However, on switching to the long-loop limit in Eq. (21) we find the surprising result

$$N(L \gg d^2/a) \simeq \frac{a}{L}\left(1 + 6e^{-2\pi^2aL/3d^2} + \cdots\right). \tag{26}$$

That is, for long strings $N(L)$ behaves like L^{-1}. This is the phase we invoked in the introduction, with a natural description in terms of nonzero winding number, i.e., all strings with nonzero winding number "wrap" themselves around the lattice. The appearance of this phase is a direct consequence of the periodiciy of our boundary conditions. With the infinite boundary conditions used in the earlier work on strings this phase is not present because there is a finite probability of a string not returning to its starting point, and hence being infinite [13]. Instead, on a periodic lattice the probabiliy of return is always unity—given a sufficiently long random walk, and hence *all* strings form loops.

Figure 1 shows the predicted loop distribution of orientable loops for a 40^3 periodic lattice. Although $N(L)$ is given by the product of three infinite sums, the long-loop distribution converges very rapidly and is essentially one term. The short-loop distribution converges more slowly, though we still see good numerical convergence of the untransformed theta functions with as few as five terms. Both short- and long-loop regions are clearly in evidence, separated by a characteristic length scale l_c.

Following Allega, Fernández, and Taracón [5], we determine l_c from

$$N_{L\ll d^2/a}(l_c) \simeq N_{L\gg d^2/a}(l_c). \tag{27}$$

To lowest order this gives

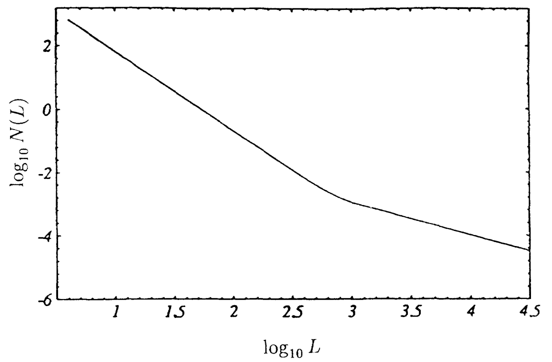

FIG. 1. Loop distribution for a periodic cubic lattice with 40^3 points. The two "phases" of short and long loops, separated by a new scale l_c, are clearly visible.

$$l_c \simeq \frac{3d^2}{2\pi a} \tag{28}$$

showing the expected dimensional dependence for Brownian strings.

Comparing our Fig. 1 with Fig. 1 of Ref. [5] shows that our theory is in remarkable agreement with the simulations. We predict approximately 3% more loops on small scales, though given our original naïve incorporation of backtracking this is to be expected. At the phase transition the effective string tension (which included the backtracking effects) vanishes. Hence at T_s backtracking is not entirely accounted for. Further comparisons reveal that our predictions for l_c also agree well, the factor $3/2\pi$ being 15% lower than the numerical values. This discrepancy is easily explained by noting that the precise $N(L) \propto L^{-5/2}$ result is only valid in the infinite d limit. Had we considered extra terms we would have found that the true dependence is roughly $L^{-2.4}$. Thus the slope of $N(L)$ in the short-loop phase is shallower and the intersection scale l_c increased.

Consider now the nature of the loops formed at the phase transition. Clearly strings of length greater than $O(d^2/a)$ will typically come into contact with one of the boundaries — and hence have a nonzero winding vector $\mathbf{u}'$. Having decomposed $N(L)$ into a sum over the winding vector $\mathbf{u}'$ it is important to know what contribution to the overall string density is made by both topological and nontopological string; that is, string which does and does not wind around the lattice, respectively. Setting $l' = m' = n' = 0$, we see from (22) that

$$n_{\mathbf{0}} = \frac{d^3}{a^2 L}\left(\frac{3a}{2\pi L}\right)^{3/2}, \tag{29}$$

implying that almost all short loops have a zero winding vector. Moreover, this is identical to the number of loops in the subvolume d^3 of an infinite lattice (16). The corresponding topological contribution to the total loop distribution is just the right-hand side of (22) minus this number. [We have implicitly assumed that there are *no* short loops with a nonzero winding number, which is only true in the limit as d becomes large and the exponential factor in (25) negligible.] In the long string limit we can use the approximation

$$\lim_{aL \gg d^2} \vartheta\left(0 \,\middle|\, \frac{3id^2}{2\pi aL}\right) - 1 \simeq \left(\frac{2\pi aL}{3d^2}\right)^{1/2} \operatorname{erfc}\left(\frac{3d^2}{2aL}\right)^{1/2}, \tag{30}$$

which gives the topological string distribution

$$n_{\mathbf{u}'\neq\mathbf{0}}(L) \simeq \frac{a}{L}\left[1 - \frac{3}{\sqrt{\pi}}\left(\frac{3d^2}{2aL}\right)^{1/2} + \frac{6}{\pi}\left(\frac{3d^2}{2aL}\right) - \frac{2}{\sqrt{\pi}}\frac{4-\pi}{\pi}\left(\frac{3d^2}{2aL}\right)^{3/2} + \cdots\right]. \tag{31}$$

On comparing (31) with (26) we note that almost all long strings will have some topological winding around the lattice. Moreover, the difference between (31) and (26) is the number of long strings which do *not* come into contact with the boundaries.

Since we now know the distribution of string lengths we can calculate the fraction that topological string makes to the overall string density Λ, defined by

$$\Lambda = \Lambda_{\mathbf{0}} + \Lambda_{\mathbf{u}'\neq\mathbf{0}} \simeq \left(\frac{a}{d}\right)^3 \left\{\sum_{4}^{l_c/a} L n_{\mathbf{0}}(L) + \sum_{l_c/a}^{\kappa(d/a)^3} L n_{\mathbf{u}'\neq\mathbf{0}}\right\}, \tag{32}$$

where we have assumed that all intermediate strings ($L \simeq d^2/a$) have a nonzero winding number. The upper limit on L is calculated from a threshold fraction of the total volume of the lattice κ, above which the system can be considered full of string — above this limit the fields are no longer in stringlike configurations and the unbroken symmetry of the system will be restored. We would like to determine κ analytically. It is easy to understand from where it emerges and how it is constrained. Unfortunately it is not so easy to determine its precise value.

Suppose we have a box full of fundamental string with zero thickness. Clearly, the total number of links that could be covered with string is $(d/a)^3$, which means that $\kappa \leq 1$. We might expect κ to have some weak dependence on box size (d/a). This is motivated by the case of a self-avoiding random walk beginning at the origin [17]. The fraction $\bar{\kappa}$ of space accessible to the walk, treated as a non-self-avoiding random walk in self-consistent impenetrable dust, behaves with volume as $\bar{\kappa} = 1 - O((d/a)^{4/3})$. The simulations of [3–5], whose work is concerned principally with U(1) string formation, provides values of κ in the region of 0.7 for lattices smaller than about 100^3 points.

Defining $f_t(d,\kappa)$ as the fraction of topological string for a given lattice size, $f_t = \Lambda_{\mathbf{u}'\neq\mathbf{0}}/\Lambda$, in the infinite d limit this tends to the nonzero ratio

$$\lim_{d\to\infty} f_t(d,\kappa) = \frac{\kappa}{\kappa + \Lambda_{\mathbf{0}}}, \tag{33}$$

where to leading order

$$\Lambda_{\mathbf{0}} = \Lambda_\infty = \left(\frac{3}{2\pi}\right)^{3/2}. \tag{34}$$

For κ of 0.7 this result implies that about 68% of loops formed at the phase transition will be topologically nontrivial. Since κ must be less than 1 there is also an upper bound on f_t of 75%. Moreover, when we consider the infinite lattice-size value of κ we find that f_t tends to the limiting value of 60% for a simple cubic lattice.

Figure 2 shows the fraction of topological string plotted against lattice size for the case of $\kappa = 0.7$. From this we see that f_t falls quite rapidly from a value of near unity to the limiting value given above. These results are once more in excellent agreement with the simulations of Allega *et al.* [4]. For very small lattices we would expect the fraction of topological string to approach unity. This feature is not completely reproduced because at these scales our approximations break down. The largest simulations currently have about 100^3 lattice points. Our results imply that they have yet to show limiting behavior and that finite-lattice effects should be small but measurable.

These results should be contrasted to those of [13] in which it is argued that, in the infinite volume limit, we should not think in terms of loops. Rather, the authors use the fact that Λ_0 is just the probability that a random walk on the lattice intersects itself. Then κ is to be understood as $1 - \Lambda_0$, the probability that a random walk does not intersect itself (i.e., becomes an infinite string). Thus $f(\infty, \kappa) = 1 - \Lambda_0$. This is certainly compatible with our results, requiring a lattice totally full of string at the transition. We do not wish to be so prescriptive in our simple model.

In conclusion we have shown how a simple model of string formation on a periodic lattice can accurately predict the results of numerical simulations, and shown how it is that these results are similar to those obtained numerically in [13] using a nonperiodic lattice. Moreover, we have provided a physical interpretation of the long string region observed in the simulations on periodic lattices, namely, that the long string winds around the lattice. With this interpretation we have given the first prediction of how the total fraction of long (or toplogical) string varies with lattice size and deduced that the simulations are not yet large enough to show asymptotic behavior. This new phase for extremely long strings is an artifact of the periodicity and would not necessarily be expected for more general boundary conditions.

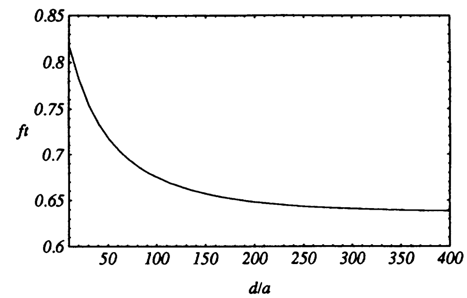

FIG. 2. Fraction of topological string formed on a cubic lattice with $(d/a)^3$ points. We have chosen $\kappa = 0.7$ in accordance with the simulations of [4–6].

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