Interactions between topological point singularities

S. Ostlund
Laboratory of Atomic and Solid State Physics, Clark Hall, Cornell University, Ithaca, New York 14853
(Received 5 February 1981)

The interaction between point singularities is investigated as a function of dimension d for the isotropic $n = d$ fixed length spin model. For dimensions greater than or equal to 3, the region of d-dimensional space which is perturbed by the pair of singularities collapses into a string joining the two singular cores. Thus the interaction between point singularities in the three-dimensional (3D) classical Heisenberg model ($n = d = 3$) is radically different from the interactions between vortices in the 2D XY model ($n = d = 2$).

The importance of the possibility of having vortices in the two-dimensional (2D) XY model has been recognized for almost eight years. Since the work of Kosterlitz and Thouless,[1] the consequences of the ideas of vortex-mediated melting in the XY model have led to a thorough understanding of 2D systems in which vortexlike excitations cause the melting.[2] In contrast, very little is known about the role of topological point defects, the higher-dimensional analog of vortices in the 3D classical Heisenberg model.[3] The reason the XY model has been so successfully studied, while little progress has been made for the 3D case, is that for the XY model, the nonlinearities associated with the constraint that the spin $\vec{s}$ have length unity can be removed by representing the spin by an angle field. In contrast, the nonlinearities in the 3D model cannot be removed by such a trick.

The 2D XY or 3D Heisenberg models are members of the class of models with the Hamiltonian in d-dimensional space given by

$$H = \tfrac{1}{2} J \sum_{ij} \int d^d r \, \frac{\partial s_i}{\partial r_j} \frac{\partial s_i}{\partial r_j} \quad , \tag{1}$$

where the summation is over the d indices of $\vec{r}$ and the n indices of $\vec{s}$. The vector $\vec{s}$ is constrained to have length unity: $\vec{s}^{\,2} = 1$. In the rest of this paper the equality ($n = d$) is assumed.

An example of a point singularity in the 3D Heisenberg model occurs at a position $\vec{r}$ from where all the spins point radially outward. Similarly, a vortex is a point singularity in $d = 2$. These point singularities are called topologically stable because no local fluctuation in a uniform system can produce such a singularity. Furthermore, imposing uniform boundary conditions at infinity forces the singularities to occur in oppositely charged pairs.

Halperin has suggested that an understanding of the interaction between point defects may be relevant to the understanding of the critical behavior in the 3D Heisenberg model.[2] More generally, Cardy and Hamber have discussed renormalization-group relations for the Hamiltonian in Eq. (1.1) as a set of analytic equations in n, d, the coupling constant J, and a parameter y which reduces to the vortex fugacity for $n = d = 2$.[4] They find that close to $d = 2$ there is a curve in nd space such that for $n \leqslant n_c(d)$ the fugacity of topological defects must be considered explicitly. They also suggest that $n_c(d) \geqslant d$. If this is the case, the present work may be relevant to an eventual theory of critical behavior of the 3D Heisenberg model. The relevance of ϵ-expansion renormalization-group techniques to $n = d = 3$ is currently a topic of debate.[2,4–6]

In the present work, the nature of the interaction between two topological point singularities is explored as a function of dimension. The region of physical space which is affected by the presence of a pair of topological point defects is found to collapse into a string in dimension greater than or *equal to* 3, so that $d = 3$ is found to be a crossover dimension where the interactions between point defects become singular. The analysis suggests that connecting the point defects pairwise by straight strings in such a way as to minimize the total string length represents a solution to the minimization of the Hamiltonian in Eq. (1) in the presence of an arbitrary number of point defects of charge ± 1 and total charge zero. The argument is not certain, however, since the analysis shows this solution only is extremal, and a more complicated many-body solution which has lower energy cannot be excluded. At finite temperature for $d = 3$, there may be important scale-invariant fluctuations which cause the string diameter to fluctuate. Higher-order terms added to the Hamiltonian in Eq. (1) also become important for $d \geqslant 3$ for any lattice model which reduces to this Hamiltonian in the long-wavelength limit.

The value of the charge of a point singularity counts the number of times and the sense in which the spins on a $(d-1)$-dimensional surface surrounding the defect cover the order-parameter space determined by $\vec{s}^{\,2} = 1$.

Consider a very large (infinite) system with the boundary condition that the spins be uniform at the surface. It is easy to see that the interactions between defects at a finite separation must be finite since a pair of oppositely charged defects can always be enclosed in a finite d-dimensional box on which the spins are uniform on the surface. By dimensional arguments,[7] any spin configuration which minimizes energy and is singular only at the positions of the singularity must have an energy as a function of defect separation R given by

$$E(R) = JC(d)R^{d-2}/(d-2) \quad , \tag{2}$$

where $D(d)$ is a function of dimension. (The interaction is logarithmic in precisely $d=2$, where the dimensional argument above cannot distinguish between a constant function and a logarithm.) The function $C(d)$ has the value 2π for $d=2$ and will be shown to have the value 4π for $d=3$. The defects are then expected to be linearly bound in $d=3$.

Equation (2) fails for $d>3$, because the field lines can lower their energy by collapsing into a singular string. Since there is then only a core energy per unit string length, the energy as a function of defect separation will remain linear rather than increasing more rapidly as R^{d-2} as Eq. (2) would imply. The dimension $d=3$ is therefore a marginal dimension in this sense.

It will be useful to consider the point singularities of charge -1 in $d=3$ defined by

$$\vec{s}(x,y,z) = (x,y,-z)/(x^2+y^2+z^2)^{1/2} \tag{3}$$

rather than $\vec{s}(\vec{r}) = -\vec{r}/|\vec{r}|$. The defect defined by Eq. (3) can be smoothly deformed into the latter type by rotating the spins by π about the z axis. The realization in Eq. (3) of a negatively charged point defect is easily generalized to any dimension. Figure 1 shows a 2D cross section of the field lines due to a pair of oppositely charged defects. The field lines lie parallel to the direction of the spins at each point, and the configuration is axially symmetric about the z axis. The spins are assumed to point along the z axis at the boundary at infinity.

The core region between two defects is defined here to be the volume in d-dimensional space inside the isoangle surface determined by $\theta = \frac{1}{3}\pi$. This core region is found to be roughly apple shaped for dimensions less than 3, and the diameter is proportional to the separation. (The words *core region* do not *necessarily* denote a singular region in this context.) The core region in Fig. 1 is outlined by the dashed isoangle lines, for example. It will be useful to define the ratio

$$D(d) = l_{\max}/R \quad , \tag{4}$$

where $l_{\max}$ is the maximum diameter of the core region and R is the separation.

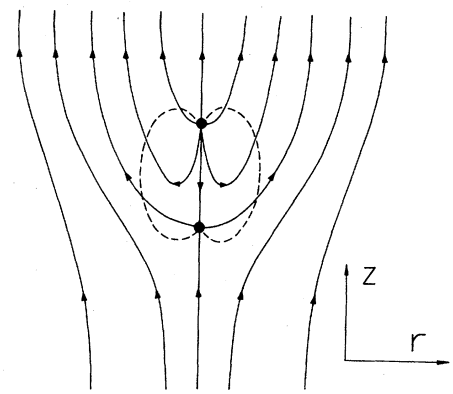

FIG. 1. Field lines parallel to the spins in a 2D cross section in the vicinity of a pair of oppositely charged topological point defects are shown. The dashed lines show the isoangle boundary of the "core region" where the spin polar angle is equal to $\frac{1}{3}\pi$. For $d \geq 3$, this core region collapses to a string.

There will be $d-2$ spatial dimensions perpendicular to the planar cross section in Fig. 1. For this particular configuration, the spin can be parametrized by only the polar angle, so that

$$\vec{s}(\vec{r}) = (\vec{r}_\perp \sin(\theta), \cos(\theta)) \quad , \tag{5}$$

where $\vec{r}_\perp$ is the $(d-1)$-dimensional unit vector of the projection of the position $\vec{r}$ onto the $(d-1)$-dimensional space perpendicular to the z axis. For $d=3$, this corresponds to ordinary axial symmetry represented by polar coordinates z and r. The angle θ is the spatial polar angle in spherical coordinates. Spherical coordinates are used for the spin, while cylindrical coordinates are used for the space. With this restriction of geometry the Hamiltonian in Eq. (1) becomes

$$H = \frac{J}{2} S_{d-2} \int r^{d-2} \left[\left(\frac{\partial\theta}{\partial r} \right)^2 + \left(\frac{\partial\theta}{\partial z} \right)^2 + \frac{d-2}{r^2} \sin^2(\theta) \right] dr\, dz \quad , \tag{6}$$

where S_{d-2} is the surface area of the $(d-2)$-dimensional sphere (S_{d-2} is 2π when $d=3$). By taking the variational derivative of this equation, one finds that the minimal energy solution must satisfy

$$\frac{\partial^2\theta}{\partial r^2} + \frac{\partial^2\theta}{\partial z^2} + \frac{d-2}{r}\frac{\partial\theta}{\partial r} = \frac{d-2}{2r^2}\sin(2\theta) \quad . \tag{7}$$

If a defect of charge $+1$ is placed at $z=1$ and a negative defect is placed at $z=-1$, the boundary condition to be satisfied is that θ be zero everywhere on the surface at infinity and zero on the line $r=0$ except for the interval $-1<z<1$, where θ takes the value π.

When Eq. (7) was solved numerically it was found that the core region collapsed into a singular line[8] as d approached 3 from below, so that $D(d)$ approached zero as $d \rightarrow 3$. The important result, which is the essential point of this article, is that $D(d)$ does not drop discontinuously to zero for $d > 3$, which a naive picture based on an analogy to vortices might suggest. In fact, for a large class of trial solutions for Eq. (6) it can be shown that $D(d) \propto (3-d)^{1/2}$ as d approaches 3 from below.[9]

In order to understand the structure of the core region in $d = 3$ more clearly, consider a plane perpendicular to the string, in the middle and far from either end at a length scale small compared to the string length. The angle θ is then just a function or the radius r. Equation (7) can then be solved exactly. One finds

$$\theta(r) = \pi - 2\arctan(\lambda r) \quad , \tag{8}$$

where λ is an arbitrary constant reflecting the scale invariance of the differential equation. (The solution was derived by noticing that the substitution $r = e^s$ leads to a sine-Gordon equation in the parameter s. The parameter λ is related to the arbitrary position of the sine-Gordon kink in an infinite system.) The energy per unit string length is then calculated to be $4\pi J$.[10]

This is a surprising result. The energy of an isolated point defect in the center of a spherical volume of physical space of radius R has energy $4\pi JR$, assuming a spherically symmetric spin configuration. The same energy is obtained if the field lines which emanate from the singularity forms a string which goes straight to the surface.

Since there is radial scale invariance in the solution to $\theta(r)$ in a z-independent cross section through a string in $d = 3$, why do the isoangle lines emanating from the defect's collapse into a string of zero diameter rather than remain finitely separated? Since the area of the unit disk around the origin occupies a large fraction of a cross section in low dimension, it is advantageous to let the angle vary relatively slowly at small radius and have a majority of the angular change at large r in order to minimize the energy of a z-independent cross section for $d < 3$. Introducing a pair of point defects at either end of the string forces the isoangle lines to converge at the ends. If the angle θ remains large at large radii, there will be a large energy cost in the curvature along the z direction when the lines must eventually converge. This competition between the tendency for a pair of defects to pull the isoangle lines together to form a string and the tendency for a z-independent solution to favor isoangle lines at large r causes the apple-shaped core region for $d < 3$. When $d = 3$, the appearance of the radial scale invariance now implies that a string configuration of any diameter has minimal energy, and the presence of the singularities at the ends compresses the string to zero diameter.

This argument suggests that local fluctuations in the string diameter are important low-energy excitations in $d = 3$. The question of the role of these in a statistical mechanical ensemble is not known. String diameter fluctuations are not expected to be important for $d < 3$, since the energy per unit length string length is minimized by a string of zero diameter and the point singularities at the end do not help to compress the string further.

The relevance of the singular string solution shows that higher-order terms added to the Hamiltonian in Eq. (1) must be considered in order to understand a lattice realization of the continuum Heisenberg model. Incorporating these, we see that terms such as $u_4(\nabla\theta)^4 + u_6(\nabla\theta)^6$ must be added to the integrand in Eq. (6). First, consider the case $u_4 > 0$. In this case, u_6 can be ignored. For $d > 3$, the parameter u_4 will determine the string diameter. For $d = 3$, the previous arguments apply and the presence of a pair of point defects again form an apple-shaped core region. Since there are now two more gradients associated with the extra u_4 term, minimizing the energy for a large class of trial solutions, one finds a core region diameter which scales like $u_4^{1/4}R^{1/2}$, where R is the defect separation.[11] If $u_4 < 0$, a radically different situation occurs for $d = 3$. It is then favorable to have a string diameter given by $(-u_4/u_6)^{1/2}$. The string diameter is then determined locally and is stiff against diameter fluctuations. The core region diameter is independent of defect separation if R exceeds this characteristic length. When $d > 3$, and $u_4 < 0$ and $u_6 > 0$, the string is also stiff against diameter fluctuations in this sense, as it is for $u_4 > 0$. Thus u_6 does not seem important for $d > 3$.

It should be emphasized that the string is not a topologically stable structure. A string configuration may relax by breaking, creating a series of short "dipole" strings. The higher-order terms may provide a core energy for the point singularity which keeps the process of subdivision from continuing to arbitrarily small scales.

ACKNOWLEDGMENTS

I would like to thank Jason Ho, Michael Peskin, and David Mermin for very useful discussions. This research was carried out through the facilities of the Materials Science Center at Cornell under NSF Grant No. DMR-79-24008.

[1]J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).

[2]For a review of the statistical mechanics of topological defects, see B. I. Halperin, in lecture notes for the *Advanced Summer Institute on Physics of Defects at Les Houches, August 1980* (North-Holland, Amsterdam, 1980). The point singularities discussed here have often been called "hedgehogs."

[3]For a review of the classification of topological defects, see N. D. Mermin, Rev. Mod. Phys. 51, 591 (1979).

[4]J. L. Cardy and H. W. Hamber, Phys. Rev. B 21, 3976 (1980).

[5]E. Brezin and J. Zinn-Justin, Phys. Rev. B 21, 3976 (1980).

[6]D. J. Amit, S. K. Ma, and R. K. P. Zia (unpublished).

[7]Assume a configuration which minimizes the energy associated with two point singularities separated by a distance a is given by $\vec{s}_a(\vec{r})$ and has energy $E(a)$. Then $\vec{s}_{\lambda a} = \vec{s}_a(\vec{r}/\lambda)$ minimizes the energy for a pair of defects a distance λa apart, since Eq. (1) is invariant under a scale change except for rescaling J. The energy associated with $\vec{s}_{\lambda a}(\vec{r})$ is easily seen to be $\lambda^{d-2}E(a)$ and Eq. (2) follows.

[8]When the algorithm was used for $d = 3$, the numerical solution corresponded to $\theta = 0$ everywhere except as specified on the boundary. This remained true for arbitrarily fine-mesh size used in the numerical solution. In fact, it is easily shown that for arbitrary $\theta(r,z)$ the function $\theta(r/D,z)$ has lower energy if $D < 1$, proving that a string solution minimizes the energy for $d \geq 3$.

[9]The trial solution is chosen to be of the form $\theta(r/D,z)$ where $\theta(r,z)$ is arbitrary but fixed as d is varied. The value of D as a function of d which minimizes the energy then can be seen to scale like $(3-d)^{1/2}$. The argument that this scaling relation is true for the function which truly minimizes the energy as a function of d is not rigorous.

[10]This solution corresponds to the "instanton" solution in the $n = 3$, $d = 2$ classical Heisenberg model discussed by A. A. Belavin and A. M. Polyakov JETP Lett. 22, 245 (1975) [Pis'ma Zh. Eksp. Theor. Fiz. 22, 503 (1975)].

[11]This proportionality is easily obtained for any trial function of the form $\theta(r/D,z)$. As u_4 is varied, the value of D which minimizes the energy is proportional to $u_4^{1/4}$, so that $D \propto u_4^{1/4} R^{1/2}$ by dimensional arguments.