Macroscopic solitons in thermodynamics

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We examine semiclassically the ϕ^4 theory in three space dimensions, and relate the circumstances which allow its macroscopic kinks to arise spontaneously in the system.

Solitons have gained a central position in many branches of condensed-matter physics.[1-9] They appear for example in the treatment of incommensurate systems,[2-5] as textures in liquid ^{3}He,[6] and as the basic ingredient of a microscopic theory of superfluid ^{4}He.[7,8] The possibility that solitons work as Bloch walls, breaking up a given system into locally ordered domains, has also been considered.[7-9] Here, we study the reason why macroscopic planar solitons can naturally sprout in the thermodynamics of three-dimensional fluids. To this purpose we analyze the kinks described by the Hamiltonian density

$$\frac{1}{2}(\dot{\phi})^2+\frac{1}{2}(\vec{\nabla}\phi)^2-\frac{m^2}{2}\phi^2+\frac{\lambda}{4}\phi^4+\frac{m^4}{4\lambda} \qquad (1)$$

in three space dimensions. ϕ is a real boson field, and $\phi \leftrightarrow -\phi$ symmetry is spontaneously broken.

As noticed by Krumhansl and Schrieffer,[10] in one dimension, where the kink has finite energy, it does occur in thermodynamics at every temperature. Three-dimensional solitons are, on the other hand, infinite sheets of infinite energy, and, at first sight, one may think they do not play any thermodynamic role. However, the presence of a soliton induces modifications in the fluctuation spectrum, and the consequent change of entropy gives life to the macroscopic sheet, above a critical temperature $T_c(\lambda)$.

Our aim is to verify the existence of this critical temperature and to compute it in a semiclassical scheme. At temperatures larger than $T_c(\lambda)$

$$F_{\text{sol}}+F^1_{\text{exc}} < F_{\text{vac}}+F^0_{\text{exc}} \ , \qquad (2)$$

where $F_{\text{vac}}=0$ and $F_{\text{sol}}=E_{\text{sol}}$ are, respectively, the vacuum and the soliton energies; F^0_{exc} is the vacuum excitation free energy, whereas F^1_{exc} is the excitations free energy on the state that contains a kink. This decomposition $F_{\text{sol}}+F_{\text{exc}}$ has been done in Ref. 10. Whenever inequality (2) holds, the macroscopic sheets are statistically favored and the system goes to a phase of solitons.

The analysis presented below, although showing the spontaneous generation of planar solitons, does not yet provide a clue to the problem of counting solitons. To know how many kinks exist at a given temperature $T > T_c(\lambda)$, one must know first how they interact, and this is a very hard nonlinear problem. The treatment of separate solitons done here certainly holds in a small vicinity of the critical point, as argued by Bak *et al.*[3] and Pokrovsky and Talanov,[4] in the context of incommensurate-systems theory. But unfortunately the number of kinks, such an important quantity, is still missed.

If x is a particular coordinate, then

$$\phi_{\text{sol}}=\frac{m}{\sqrt{\lambda}}\tanh\left(\frac{mx}{\sqrt{2}}\right) \ , \qquad (3)$$

represents a soliton at rest, parallel to the (y,z) plane. In the classical theory, the energy it contains per unit of area is

$$\sigma_{\text{class}}=\frac{2}{3}\sqrt{2}\frac{m^3}{\lambda} \ . \qquad (4)$$

Dashen, Hasslacher, and Neveu[11] (DHN) and Goldstone and Jackiw[12] carried out the semiclassical quantization of the one-dimensional version of Hamiltonian (1). This semiclassical approach is reliable for small values of λ ($\lambda << m^2$ in one dimension, and $\lambda << 1$ in three dimensions). By following the method of DHN we computed the first quantum correction to σ_{class} in three space dimensions:

$$\sigma_{\text{quant}}=\frac{m^3}{24\pi}\left[\frac{9\sqrt{2}}{\pi}-\left(\frac{3}{2}\right)^{1/2}\right]=0.0375m^3 \ . \qquad (5)$$

The three-dimensional ϕ^4 theory is not superrenormalizable, so that coupling-constant renormalization is an additional complication in getting σ_{quant}. The numerical results we present further are not much affected by the quantum correction, because we limit ourselves to the region $\lambda << 1$, where the semiclassical scheme can be trusted.

Before continuing to analyze the soliton thermodynamics, we define the theory in a box of volume $V=AL$, where A is an area parallel to the soliton sheet. Let us also consider periodic boundary conditions.

If no solitons exist, $\phi_{\text{vac}} = \pm m/\sqrt{\lambda}$, and the free energy will be (as usually, take $\beta = 1/k_B T$)

$$F_{\text{vac}} + F_{\text{exc}}^0 = k_B T V \int \frac{d\vec{p}}{(2\pi)^3} \times \ln\{1 - \exp[-\beta(p^2+2m^2)^{1/2}]\} \ , \tag{6}$$

because the energy of an elementary particle of momentum $\vec{p}$ is $(p^2+2m^2)^{1/2}$.

When the system contains one soliton, the spectrum changes as follows:

(i) There exist two classes of excitation bound to the soliton. Let $\vec{k}$ be a two-dimensional momentum vector, parallel to the kink surface. The energies of the bound excitations are $|\vec{k}|$ for the first set, and $(k^2+\frac{3}{2}m^2)^{1/2}$ for the second one. Notice that the first set of bound states is related to the zero-frequency mode of the one-dimensional theory, and the other set is associated with the mode of frequency $\sqrt{3/2}m$.[11,12]

(ii) The density of states in the continuum is also modified by the kink.[11] Let us define q as the excitation momentum orthogonal to the kink surface. q is the x momentum. Once momenta $\vec{k}$ and q are given, the energy of an unbound excitation is $(k^2+q^2+2m^2)^{1/2}$. The requirement of periodic boundary conditions implies[11]

$$Lq_n + \delta(q_n) = 2\pi n \ , \tag{7}$$

where n is an integer, and $\delta(q)$ is the phase shift of an unbound excitation with x momentum q, scattered by the soliton (recall that in this theory there is no reflection in the kink),[12]

$$\delta(q) = 2\pi - 2\arctan\left(\frac{\sqrt{2}q}{m}\right) - 2\arctan\left(\frac{q}{\sqrt{2}m}\right) \ . \tag{8}$$

Besides, if m and l are the quantum numbers of y and z directions, then

$$\sqrt{A}\,k_{ym} = 2\pi m \ , \tag{9a}$$

$$\sqrt{A}\,k_{zl} = 2\pi l \ . \tag{9b}$$

In the semiclassical treatment adopted here, quasiparticles interact with the soliton, but do not interact among themselves[12]; so, the excitation's statistical mechanics is exactly solvable.

We are now in a position to write explicitly the one-soliton-system free energy, $F_{\text{sol}} + F_{\text{exc}}^1$. F_{sol} is the contribution of the soliton itself (i.e., the one-soliton-sector free energy before we consider the fluctuation's contribution)

$$F_{\text{sol}} = A(\sigma_{\text{class}} + \sigma_{\text{quant}}) \ . \tag{10}$$

Owing to the change in the excitation spectrum, F_{exc}^1 differs from F_{exc}^0

$$F_{\text{exc}}^1 = B_1 + B_2 + U \ , \tag{11}$$

where B_1 and B_2 refer to the two sets of bound states

$$B_1 = k_B T A \int \frac{d\vec{k}}{(2\pi)^2} \ln[1 - \exp(-\beta|\vec{k}|)] \ , \tag{12a}$$

$$B_2 = k_B T A \int \frac{d\vec{k}}{(2\pi)^2} \ln\{1 - \exp[-\beta(k^2+\tfrac{3}{2}m^2)^{1/2}]\} \ , \tag{12b}$$

and U is the contribution of the unbound particles

$$U = k_B T \sum_{nml} \ln\{1 - \exp[-\beta(k_{ym}^2 + k_{zl}^2 + q_n^2 + 2m^2)^{1/2}]\} \ . \tag{13a}$$

According to Eqs. (7) and (9), the continuum limit $(L, A \to \infty)$ leads to the replacements

$$\sum_{ml} \to \frac{1}{4\pi^2} \int A\, d\vec{k} \ ,$$

and

$$\sum_{n} \to \frac{1}{2\pi} \int dq\,(L + d\delta/dq) \ ,$$

the phase-shift derivative being

$$\frac{d\delta}{dq} = -2\sqrt{2}m\left(\frac{1}{q^2+2m^2} + \frac{1}{2q^2+m^2}\right) \ .$$

In this limit, the unbound particles contribution can thus be written as [see Eq. (6)]

$$U = F_{\text{vac}} + F_{\text{exc}}^0 - k_B T A \frac{2\sqrt{2}m}{(2\pi)^3} \int d\vec{k}\,dq \left(\frac{1}{q^2+2m^2} + \frac{1}{2q^2+m^2}\right) \ln\{1 - \exp[-\beta(k^2+q^2+2m^2)^{1/2}]\} \ . \tag{13b}$$

Combining Eqs. (10)–(13), one gets the free-energy corresponding to one soliton $[Af_s(T)]$:

$$Af_s(T) = (F_{\text{sol}} + F_{\text{exc}}^1) - (F_{\text{vac}} + F_{\text{exc}}^0) = A[\sigma_{\text{class}} + \sigma_{\text{quant}} - k_B T(G_1 + G_2)] \ , \tag{14}$$

where $G_1(T)$ and $G_2(T)$ are given by

$$G_1(T) = -\int \frac{d\vec{k}}{(2\pi)^2} \ln[1-\exp(-\beta k)]$$
$$+2\sqrt{2}m \int \frac{d\vec{k}}{(2\pi)^2} \int_{-\infty}^{+\infty} \frac{dq}{2\pi} \frac{1}{(q^2+2m^2)} \ln\{1-\exp[-\beta(k^2+q^2+2m^2)^{1/2}]\} , \tag{15a}$$

$$G_2(T) = -\int \frac{d\vec{k}}{(2\pi)^2} \ln\{1-\exp[-\beta(k^2+\tfrac{3}{2}m^2)^{1/2}]\}$$
$$+2\sqrt{2}m \int \frac{d\vec{k}}{(2\pi)^2} \int_{-\infty}^{+\infty} \frac{dq}{2\pi} \frac{1}{(2q^2+m^2)} \ln\{1-\exp[-\beta(k^2+q^2+2m^2)^{1/2}]\} . \tag{15b}$$

In Ref. 13, Bishop presents a quite general treatment of one-dimensional-soliton thermodynamics. There is much similarity between our calculations and those he shows. Notice for example that the fluctuation's contribution to the soliton free energy, $A(G_1+G_2)$, is the three-dimensional analog of the function σ, which appears in Eq. (44) of Bishop's paper.

If one defines $s=k^2$, $t=k^2+\frac{3}{2}m^2$, and $r=k^2+q^2+2\ m^2$, then after integration in q, it follows:

$$G_1(T) = -\frac{1}{4\pi} \int_0^{\infty} ds \ln[1-\exp(-\beta\sqrt{s})]$$
$$+\frac{1}{4\pi} \int_{2m^2}^{\infty} dr \frac{2}{\pi} \arctan\left[\left(\frac{r}{2m^2}-1\right)^{1/2}\right] \ln[1-\exp(-\beta\sqrt{r})] , \tag{16a}$$

$$G_2(T) = -\frac{1}{4\pi} \int_{3/2m^2}^{\infty} dt \ln[1-\exp(-\beta\sqrt{t})]$$
$$+\frac{1}{4\pi} \int_{2m^2}^{\infty} dr \frac{2}{\pi} \arctan\left[2\left(\frac{r}{2m^2}-1\right)^{1/2}\right] \ln[1-\exp(-\beta\sqrt{r})] . \tag{16b}$$

Now look at the following properties of $G_i(T)(i=1,2)$.

(a) $G_i(0)=0$. This is obvious.

(b) $G_i(\infty)=\infty$. To see that this is true, we observe that

$$G_1(T) > g_1(T) = -\frac{1}{4\pi} \int_0^{2m^2} dr \ln[1-\exp(-\beta\sqrt{r})] ,$$

because $(2/\pi)\arctan\sqrt{r/2m^2-1} < 1$. Hence, property (b) holds for $G_1(T)$, since $g_1(\infty)=\infty$. An analogous procedure shows that it also holds for $G_2(T)$.

(c) $G_i(T)$ *are monotonic functions.* It is easy to verify this last property by inspecting the derivatives dG_i/dT.

Because $G_i(T)$ do not depend on λ, properties (a), (b), and (c) ensure that, for every positive λ, there is a critical temperature $T_c(\lambda)$, above which the right-hand side of Eq. (14) becomes negative. In this situation the macroscopic kink has enough statistical weight to arise spontaneously in the system.

Figure 1 shows the function $T_c(\lambda)$ in the region of small λ, where the semiclassical approximation works well.

One may not conclude that the spontaneous production of solitons would lead to a catastrophe. The total number of solitons is in fact controlled by their own interactions. To gain an insight into this controlling mechanism, let us consider cubic configurations of solitons at rest, defined in a cubic box of volume L^3, and having the following properties: (a) the Nth configuration contains $3N$ solitons; (b) there are N solitons parallel to each face of the cube; (c) the distance between any soliton and its nearest

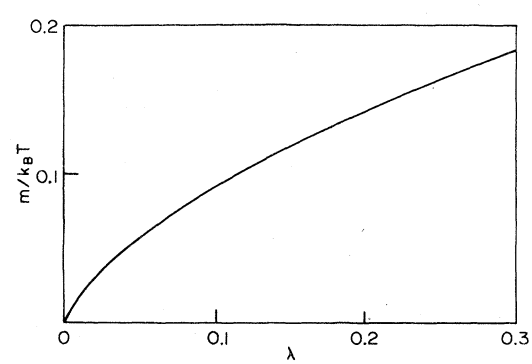

FIG. 1. The function $1/T_c$ for small values of the coupling constant λ.

parallel neighbor is always the same, $\Delta = L/N$; and (d) Δ is much larger than the soliton width, $\Delta \gg 1/m$.

Before taking into account the interactions among solitons, the free energy of the Nth configuration would be $3NAf_s(T) = 3L^3 f_s(T)/\Delta$ (recall that $A = L^2$). Now, for simplicity, let us suppose that interactions occur only over the lines where solitons cross. Therefore, the interaction between two perpendicular solitons amounts to a positive energy proportional to the length of the crossing line $:\alpha L$. Since there are $3N^2$ crossing lines, the total interaction energy is $3N^2 L\alpha = 3L^3\alpha/\Delta^2$. Therefore, the free energy of such a system will be

$$3L^3(f_s(T)/\Delta + \alpha/\Delta^2) \quad . \tag{17}$$

This expression is obviously incomplete, because we had discarded some interactions between solitons (the interaction between parallel solitons, for instance). But it serves well to illustrate the mechanism which forbids the solitons' collapse. The total number of solitons is given by $3N_0 = 3L/\Delta_0$, where Δ_0 is the value of Δ which minimizes expression (17). Above T_c, $f_s(T)$ is negative, so that, were it not for the positive interaction term α/Δ^2, we would have $\Delta_0 = 0$ (which means $N_0 = \infty$). The role of the interaction term is thus to keep Δ_0 finite, and, as a consequence, the number of solitons proportional to the box length. In summary, the quantum fluctuations make the system produce solitons, and the interactions among them forbid the system collapse.

By examining the relativistic ϕ^4 theory, we verified that macroscopic solitons indeed appear naturally in three-dimensional systems, by virtue of the distortions they provoke on the excitation spectrum. This result has probably a quite general character, and can, we think, be extended to most theories exhibiting solitons.

In a previous paper,[8] studying the microscopic theory of superfluidity (the nonrelativistic $|\phi|^4$ theory), we had already reached the same conclusion. However, the calculations of that paper suffer from two deficiencies we overcome here: there, the modifications on the density of unbound state are not taken into account, and the bound-state energies are obtained by means of a variational approach. Besides, instead of a unique type of kink, that theory has a continuum family of different solitons, which makes its treatment more difficult.

Recently, Wallace and Zia[14] studied the statistical mechanics of an interface between two discrete thermodynamic phases. Their field f, representing the deviation from planar of an essentially sharp interface, is a field of *bound* excitations. The ϕ^4 kink is analogous to this interface, and our analysis stresses the need of considering changes in the density of *unbound* excitations as well.

The spectrum modifications caused by solitons are particularly important in the microscopic theory of superfluidity,[7,8] where we noticed a great similarity between the set of bound excitations and the spectrum of liquid ^{4}He, obtained in neutron scattering experiments.

The study of soliton thermodynamics has been developing rapidly. As an example, we mention the papers by Maki and Takayama,[15] which deal with some one-dimensional theories, including the ϕ^4 model, whose three-dimensional version is discussed here.

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