Solitonic bubbles and phase transitions

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It is shown that the nontopological bubble-shaped classical solutions which are possible in a scalar field theory with quartic and sextic self-interactions in $1+1$ dimensions are responsible for the discontinuous transition in the quantum problem between a phase with a degenerate excited level and a disordered one.

A study of the real scalar field theory with quartic and sextic self-interactions in $1+1$ dimensions had shown[1] that for lateral wells of the potential deeper than the central one a static classical solution with a discontinuous derivative of bubble type appeared in addition to kink solitons. In the lattice version of the model these bubble states were considered among the quantum excitations for the ordered phase.

More recently[2] it has been seen that the nonlinear Schrödinger equation coming from a Lagrangian with a three-well potential possesses solutions corresponding to the above ones in the static case, such that those with a continuous derivative are solitonic kinks when the lateral wells are the absolute minima and they are of bubble type for central absolute minimum. These latter solutions have been shown to be unstable in the static case for all dimensions and to acquire stability above a critical velocity at least in 1 and 2 spatial dimensions. This nonlinear Schrödinger equation appears in models for superfluidity,[3] defectons,[4] ferromagnetic chains with deformations,[5] molecular chains with vibrations,[6] propagation of light in nonlinear medium,[7] and heavy-ion collisions with Skyrme interactions.[8]

In this paper we show that for the quantum lattice version of the Klein-Gordon model, the kink and bubble excitations in the ordered phase are capable of explaining with a simple perturbative treatment the phase diagram which had been obtained in Ref. 1 by renormalization-group techniques. While kink-type excitations are responsible for the second-order transition to the disordered phase, condensation of bubbles produces quite accurately the first-order transition to a phase where the first excited level is degenerate. The Klein-Gordon model has several applications in condensed matter,[9] and in particular the tricritical point[10] of the He^3-He^4 mixture is correctly reproduced by our treatment.

It must be noted that our solitonic bubbles, which correspond to a localized spatial region of a vanishing field inside an ordered ground state, are somehow complementary to the nontopological solitons[11] which are regions of a nonvanishing field in an unbroken ground-state medium and have interesting applications in cosmology.[12]

Starting from the $(1+1)$-dimensional model,

$$\mathcal{L}=\tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi-U(\phi) \tag{1}$$

with

$$U(\phi)=a_1\phi^6+a_2\phi^4+a_3\phi^2\ ,$$

where $a_1,a_3>0$ and $a_2<0$, its lattice quantum Hamiltonian version restricted to the three lowest levels in each site j is[1]

$$H=\sum_{j=1}^{N}\left[\begin{pmatrix}0&0&0\\0&-\epsilon&0\\0&0&-K\end{pmatrix}_j -\Delta\begin{pmatrix}0&1&0\\1&0&\alpha\\0&\alpha&0\end{pmatrix}_j\begin{pmatrix}0&1&0\\1&0&\alpha\\0&\alpha&0\end{pmatrix}_{j+1}\right]\ , \tag{2}$$

where $\alpha=[\epsilon/(K-\epsilon)]^{1/2}$ and Δ is related to the matrix element of ϕ_j between neighboring levels.

The use of the renormalization group (RG) leads to the phase diagram of Fig. 1. Phase I corresponds to a nondegenerate ground state and a degenerate excited level, phase II is a disordered one with three nondegenerate

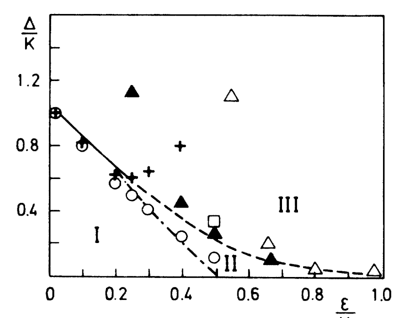

FIG. 1. Phase diagram of three-level chain model in Eq. (2). The dashed curve corresponding to a second-order transition and the solid and dashed-dotted curves showing discontinuous transitions are obtained by the block-spin method of Ref. 1. Open triangles show kink condensation and solid triangles its spin-$\frac{1}{2}$ approximation according to the perturbative treatment of Eqs. (9) and (12). Open circles denote bubble condensation and crosses bubble-kink condensation according to Eqs. (15) and (17). The open square is the degenerate kink and bubble-kink condensation due to Eq. (13).

states, and phase III is the ordered one with a double-degenerate ground level.

In terms of effective classical potentials $U_{\rm eff}(\phi)$, the above results may be visualized according to Fig. 2. Phase I is described by $U_{\rm eff}$ (a) where the ground state is given by the deepest well and the degenerate excited states by the secondary minima. Phase II corresponds to three nondegenerate levels of the single well (b) and phase III is characterized by the degenerate ground states of the two deepest wells and by the secondary minimum of (c) as an excited state.

According to Ref. 2, for the case (c) there are classical solutions which start from the left well for $x\to-\infty$ and end in the right one for $x\to+\infty$ corresponding to solitonic kinks which tend to disorder the system. For decreasing Δ/K and $\epsilon/K>0.2$, the kink condensation makes the barrier separating these wells disappear giving a continuous transition to the disordered phase II. When $\epsilon/K<0.2$ the central well becomes the absolute minimum before the barrier disappears passing to the situation (a) with a discontinuous transition.

For $\epsilon/K<0.5$ as shown in Ref. 2 there are classical solutions of bubble type which start for $x\to-\infty$, e.g., from the right well of Fig. 2(a), pass to the central well, and return to the original one for $x\to\infty$. We may interpret that in phase I they tend to destroy the degeneracy of the excited level. For increasing Δ/K both the height of the lateral barriers and the depth of the central well decrease. For $\epsilon/K>0.2$ bubbles succeed in making the former disappear first, passing to the disordered phase II with a transition which is discontinuous in the sense that the expectation value of ϕ for the excited state passes from a finite to a vanishing value. For $\epsilon/K<0.2$ the central well becomes a secondary minimum before the lateral barriers may disappear producing a first-class transition to the ordered phase III with a finite expectation value of ϕ for each one of the degenerate states which now correspond to the ground level. Along this critical curve the effect of kinks and bubbles must coincide since there is a single transition in this region represented by the passage from (c) to (a).

We will show that the above intuitive scheme emerges from a perturbative calculation where the kinks and bubbles are taken in their discretized lattice version. The strategy will be to consider the lowest excitations in each parameter region, which produce transitions when they become degenerate with the ground level.

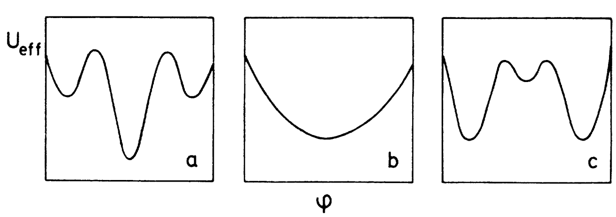

FIG. 2. Effective potentials for three-level model. (a) Nondegenerate ground level and degenerate excited one (phase I). (b) Three nondegenerate levels (phase II). (c) Degenerate ground level and nondegenerate excited one (phase III).

With a unitary transformation[1] of Eq. (2) and the subtraction of a constant, the three-level Hamiltonian may be rewritten as

$$\tilde{H}=\sum_{j=1}^{N}\left[\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}_j-\tilde{K}\begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix}_j-\tilde{\Delta}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}_j\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}_{j+1}\right], \quad (3)$$

where

$$\tilde{K}=\frac{\sqrt{2}(K-2\epsilon)}{[\epsilon(K-\epsilon)]^{1/2}},\quad \tilde{\Delta}=\frac{\sqrt{2}\Delta(1+\alpha^2)}{[\epsilon(K-\epsilon)]^{1/2}}.$$

Starting from large $\tilde{\Delta}$, the unperturbed ground state may be taken as that where all sites are in the state

$$\begin{pmatrix}1\\0\\0\end{pmatrix}$$

corresponding to energy $E_0^{(0)}$. The kink will be the state where, compared to the ground one, on the right of a certain site j all states are flipped, i.e.,

$$\begin{pmatrix}0\\0\\1\end{pmatrix},$$

giving an energy $E_K^{(0)}=E_0^{(0)}+2\tilde{\Delta}$. Bubbles correspond to a site j with

$$\begin{pmatrix}0\\1\\0\end{pmatrix}$$

between normal "spin-up" regions for all the other sites. The energy will be $E_B^{(0)}=E_0^{(0)}+2\tilde{\Delta}-\tilde{K}$ so that a bubble is degenerate with a topological state where the site j with

$$\begin{pmatrix}0\\1\\0\end{pmatrix}$$

is between a "spin-up" and a "spin-down" region which we will call bubble kink with energy $E_{BK}^{(0)}=E_B^{(0)}$. Notice that bubbles larger than one site have a higher energy provided $\tilde{\Delta}>\tilde{K}$. Therefore for $K<2\epsilon$ kinks are the lowest-lying excitations whereas for $K>2\epsilon$ this role is played by the degenerate bubble and bubble-kink states.

Apart from the case $K=2\epsilon$ where bubble states are degenerate with kink ones, there are no first-order corrections to $E_K^{(0)}$ due to the first term of Eq. (3).

Calculating the second-order perturbation corrections for decreasing $\tilde{\Delta}$, the ground state is connected only to bubbles

$$E_0^{(2)}=E_0^{(0)}-N\frac{1}{2\tilde{\Delta}-\tilde{K}}. \quad (4)$$

For the correction to the kink energy the problem is degenerate. The diagonal elements of the secular equation correspond to the connection with bubble-kink or separate one-bubble–one-kink states, whereas the nondiagonal elements appear for neighboring kinks via bubble-kink states

$$\left|\left|\left[\frac{2}{\tilde{K}}-\frac{N-2}{2\tilde{\Delta}-\tilde{K}}-\lambda\right]\delta_{jj}+\frac{1}{\tilde{K}}\left[\delta_{jj+1}+\delta_{jj-1}\right]\right|\right|=0\ . \tag{5}$$

In terms of the collective kink states

$$|k\rangle=\frac{1}{\sqrt{N}}\sum_j e^{ikj}|K_j\rangle\ , \tag{6}$$

Eq. (5) is diagonalized with eigenvalues

$$\lambda(k)=\frac{2}{\tilde{K}}-\frac{N-2}{2\tilde{\Delta}-\tilde{K}}+\frac{2}{\tilde{K}}\cos k \tag{7}$$

so that

$$E_K^{(2)}(k)=E_0^{(2)}+2\tilde{\Delta}+\frac{2}{2\tilde{\Delta}-\tilde{K}}+\frac{2}{\tilde{K}}(1+\cos k)\ . \tag{8}$$

In the region $K<2\epsilon$ where $\tilde{K}<0$ and the single-site potential of the quantum Hamiltonian is of the type (c) the transition is obtained when the kink band touches the ground level, i.e.,

$$2\tilde{\Delta}+\frac{2}{2\tilde{\Delta}+|\tilde{K}|}-\frac{4}{|\tilde{K}|}=0\ . \tag{9}$$

In the limit $K\to\epsilon$ where $|\tilde{K}|$ and $\alpha^2\to\infty$, Eq. (9) is satisfied for $\Delta\to 0$, which agrees with the RG order-disorder curve of Fig. 1. For intermediate values, e.g., $K=1.5\epsilon$, the transition according to Eq. (9) corresponds to a coupling Δ slightly higher than the RG calculation.

In this same region $K<2\epsilon$ one may assume as a good approximation to take only the two lowest levels of Eq. (2), i.e.,

$$H\simeq\sum_{j=1}^{N}\left[\begin{pmatrix}-\epsilon & 0\\ 0 & -K\end{pmatrix}_j-\Delta\frac{\epsilon}{K-\epsilon}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}_j\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}_{j+1}\right]\ , \tag{10}$$

so that an Ising model is considered. In this case no bubbles are present and first-order corrections to kink energies appear giving

$$E_K^{(1)}(k)=E_0+2\Delta\frac{\epsilon}{K-\epsilon}+(K-\epsilon)\cos k \tag{11}$$

with a transition expected for

$$\frac{\Delta}{K}=\frac{1}{2(\epsilon/K)}\left[1-\frac{\epsilon}{K}\right]^2\ , \tag{12}$$

which agrees very well with the RG curve up to $K=2\epsilon$. One has to note that the critical ratio Eq. (12) coincides with the exact result for the Ising model Eq. (10) but the latter will not be a good approximation of the three level Eq. (2) for $\epsilon/K<\frac{1}{2}$. There Eq. (12) will predict too high values of Δ as seen in Fig. 1.

For $K\sim 2\epsilon$ the second-order perturbation calculation Eq. (8) is not applicable because $\tilde{K}\sim 0$ and kinks and bubble-kink states become degenerate. A first-order calculation is done for $K=2\epsilon$ with these states[1] giving the mixed bands

$$E_{K,\mathrm{BK}}^{(1)}(k)=E_0+2\Delta\pm\sqrt{2}\epsilon\cos\frac{k}{2}\ , \tag{13}$$

which correspond to a rather good critical ratio $\Delta/K\simeq 0.35$.

For $K>2\epsilon$ the kink is no longer the lowest-lying excitation due to the fact that the single-site potential of the Hamiltonian is of type (a). Therefore for decreasing Δ the transitions will come from the degeneracy of the lower-lying bubbles and bubble kinks with the ordered ground state. With a second-order calculation, bubble and bubble-kink states are independently corrected.

For bubbles, the diagonal elements correspond to connecting them to the ground state, single-site flipped-spin states, two-site bubble states, and two single-site bubble states. All nondiagonal elements for a bubble different from the original one appear via the vacuum state. The secular equation is

$$\left|\left|\left[\frac{4-N}{2\tilde{\Delta}-\tilde{K}}-\frac{1}{2\tilde{\Delta}+\tilde{K}}-\frac{2}{\tilde{\Delta}-\tilde{K}}-\lambda\right]\delta_{jj}+\frac{1}{2\tilde{\Delta}-\tilde{K}}(1-\delta_{jj})\right|\right|=0\ , \tag{14}$$

which, for $2\tilde{\Delta}-\tilde{K}>0$, gives as lowest level the $N-1$ states with energy

$$E_B^{(2)}=E_0^{(2)}+2\tilde{\Delta}-\tilde{K}+\frac{3}{2\tilde{\Delta}-\tilde{K}}-\frac{2}{\tilde{\Delta}-\tilde{K}}-\frac{1}{2\tilde{\Delta}+\tilde{K}}\ . \tag{15}$$

On the other hand, for bubble-kink states the diagonal elements connect to kinks, two-site bubble-kink states and to one-bubble–one-bubble–kink states. The nondiagonal elements are possible only for neighboring bubble-kink states. Therefore the secular equation

$$\left|\left|\left[\frac{3-N}{2\tilde{\Delta}-\tilde{K}}-\frac{2}{\tilde{\Delta}-\tilde{K}}-\frac{2}{\tilde{K}}-\lambda\right]\delta_{jj}-\frac{1}{\tilde{K}}\left[\delta_{jj+1}+\delta_{jj-1}\right]\right|\right|=0 \tag{16}$$

gives an energy band

$$E_{BK}^{(2)}(k)=E_0^{(2)}+2\tilde{\Delta}-\tilde{K}+\frac{3}{2\tilde{\Delta}-\tilde{K}}-\frac{2}{\tilde{\Delta}-\tilde{K}}-\frac{2}{\tilde{K}}(1+\cos k)\ . \tag{17}$$

Starting from large Δ, when the lower edge of the band Eq. (17) touches the ground level, the system is disordered by bubble-kink condensation along a curve which is too high in the region around $\epsilon/K\sim 0.5$ compared to the RG separation between phases II and III but that agrees with it for intermediate values $\epsilon/K\sim\frac{1}{4}$ and reproduces very well the curve separating III and I for $\epsilon/K<0.2$.

On the other hand, the condition for degeneracy of bubble and ground state from Eq. (15) coincides accurately with the curve of Fig. 1 separating phases I and II for $0.2 < \epsilon/K < 0.5$. For $\epsilon/K < 0.2$ the curve coming from the degeneracy of bubbles and ground state becomes undistinguishable from the one caused by bubble-kink condensation. Along these curves $\tilde{\Delta} > \tilde{K}$, so that larger bubbles have energies higher than the minimal one. It must be noted that for the Δ value which corresponds to the transition coming from Eq. (15) the system is no longer ordered since the transition produced by Eq. (17) has already occurred. So our present treatment mimics the fact that bubbles cause a transition that affects the excited level and not the ground one. The tricritical point where the curves corresponding to transitions due to bubbles and bubble kinks meet, i.e., $\epsilon/K \simeq 0.2$ and $\Delta/K \simeq 0.65$, is nicely suggested by our simple perturbative treatment and agrees with the experimental result for He^3-He^4 mixture.[13]

In conclusion, apart from some computational problems related to the perturbative calculation, we may understand the passage to a disordered phase by means of topological solitons and to a phase with degenerate excited level through nontopological bubble-type solitons. In our quantum lattice treatment for intersite coupling above the critical curves, both the kink excitation for $\epsilon/K > 0.5$ and the bubble kink for $\epsilon/K < 0.5$ correspond to the classical topological soliton. On the other hand, the bubble excitation is the quantum counterpart of the classical continuous solitonic bubble for the region $\epsilon/K < 0.5$ where it exists.

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