39

Kinks in the Klein–Gordon model with anharmonic interatomic interactions: a variational approach

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We consider the nonlinear Klein–Gordon chain including anharmonic interatomic interactions. We use a direct perturbation method and a variational approach to obtain the approximate kink solutions of the model in the continuum limit taking the ϕ^4 and sine-Gordon chains as particular examples. The kink critical velocity due to the cubic anharmonicity is found analytically. Some physically important parameters of the kink, such as its effective mass and energy, are calculated based on the approximate solution and the results are checked by numerical simulations. It is demonstrated that the variational approach yields very accurate results for the kink parameters.

1. Introduction

It is well known that a number of physical systems may be described by the extended nonlinear Klein–Gordon model: a chain of interacting atoms placed in a nonlinear external potential. As examples, we would like to mention dislocations in solids [1,2], layers absorbed on crystal surfaces [3,4], hydrogen-bonded systems [5,6]. When only nearest-neighboring interactions with the energy $W(u_{n+1}-u_n)$ are taken into account, u_n being the displacement of the nth atom from an equilibrium position, the Hamiltonian of the model in the continuum approximation reduces to the form (the lattice constant is equal to unity, and dimensionless units are used)

$$H=\int_{-\infty}^{\infty} dx\,[\tfrac{1}{2}u_t^2+W(u_x)+V(u)]\,, \quad (1)$$

where $V(u)$ is the external potential, and the subscripts t and x stand for the derivatives in time and space coordinates respectively. The equation of motion derived from the Hamiltonian is

$$u_{tt}-W''(u_x)u_{xx}+V'(u)=0\,. \quad (2)$$

If the external potential $V(u)$ has at least two equivalent minima, say at $u=u_1$ and $u=u_2$ ($u_1<u_2$), so that $V(u_1)=V(u_2)=0$, then eq. (2) supports topological solitons, the so-called kinks, with the asymptotics $u(-\infty)=u_1$, $u(+\infty)=u_2$. Analogously, an antikink is defined as a solution with the asymptotics $u(-\infty)=u_2$, $u(+\infty)=u_1$.

Two important and well-known examples of the model (1), (2) are the ϕ^4 and sine-Gordon (sG) models, whose potentials $V(u)$ have the form

$$V(u)=\tfrac{1}{4}(1-u^2)^2 \quad (\phi^4 \text{ model})\,,$$
$$=1-\cos u \quad (\text{sG model})\,. \quad (3)$$

Generally, the interaction potential $W(u_x)$ may be approximated by the following expansion,

$$W(u_x)=\tfrac{1}{2}u_x^2+\epsilon P(u_x)\,, \quad (4)$$

where ϵ is a small constant parameter, and $P(u_x)$ accounts for anharmonic interatomic interactions. Note that in the special case of $\epsilon=0$ eqs. (2)–(4) reduce to the standard ϕ^4 and sG models, which admit kink solutions in the following form,

$$u_{\phi^4} = \pm\tanh[(x-vt)/\gamma] , \quad (5)$$

$$u_{sG} = 4\tan^{-1}\exp[\pm(x-vt)/\gamma] , \quad (6)$$

where

$$\gamma \equiv \sqrt{1-v^2} . \quad (7)$$

When the perturbation is included ($\epsilon \neq 0$), it is usually impossible to obtain an exact analytical solution of eq. (2), and one needs to use qualitative analysis, perturbation theory or numerical simulations (see refs. [7-12]). The purpose of this paper is to demonstrate that a variational approach may be used to obtain an approximate kink solution of eqs. (2), (4), and to calculate some important kink parameters such as the effective mass of the kink and its energy. The critical velocity of the kink in the perturbed system is also determined by the variational method, and the result is consistent with an exact formula. Comparing the results obtained by the variational method, direct perturbation approach and numerical simulations, we find that the variational approach gives very accurate results.

2. Perturbation method

Let us assume that eq. (2) has a travelling wave solution,

$$u = u(z) = u(x-vt) , \quad (8)$$

then, substituting eq. (8) into (2), we obtain the following second-order ordinary differential equation,

$$-\gamma^2 u_{zz} - \epsilon P''(u_z) u_{zz} + V'(u) = 0 . \quad (9)$$

Multiplying eq. (9) by u_z and integrating over $(-\infty, z)$ we obtain the first integral of eq. (9),

$$-\tfrac{1}{2}\gamma^2 u_z^2 - \epsilon Q + V(u) = 0 , \quad (10)$$

where

$$Q = \int_{-\infty}^{z} dz\, P''(u_z) u_{zz} u_z \equiv u_z P'(u_z) - P(u_z) , \quad (11)$$

here for the kink (antikink) solutions the integration constant is zero, because $u \to u_1$ (u_2) and $u_z \to 0$ when z tends to $\pm\infty$.

We will look for the kink solution of eq. (9) in the form

$$u(z) = u_0(z) + \epsilon\psi(z) , \quad (12)$$

where $u_0(z)$ is the kink of the unperturbed system ($\epsilon = 0$). Substituting eq. (12) into eq. (10), performing the expansion $V(u_0+\epsilon\psi) \approx V(u_0) + \epsilon V'(u_0)\psi$, and using the relationship between $u_0(z)$ and $V(u_0(z))$, we come to the following first-order equation,

$$\gamma^2 u_0'^2 (\psi/u_0')' = -Q . \quad (13)$$

From eq. (13) we can obtain

$$\psi(z) = -\frac{u_0'}{\gamma^2} \int dz \frac{Q}{u_0'^2} . \quad (14)$$

The result (14) describes a correction to the kink shape due to the anharmonic interatomic interactions. It may be used to calculate some parameters of the kink. For example, for the cubic and quartic anharmonicity,

$$\epsilon P(u_x) = \tfrac{1}{6}\alpha u_x^3 + \tfrac{1}{12}\beta u_x^4 , \quad (15)$$

we may obtain the perturbation-induced effective mass of the kink in the form

$$m_k = \int_{-\infty}^{\infty} dz\, u_z^2|_{\gamma=1} = \int_{-\infty}^{\infty} dz\, u_0'^2 - \epsilon \int_{-\infty}^{\infty} dz\, Q$$

$$= \sqrt{2} I_1 - \tfrac{2}{3}\alpha\sigma I_2 - \frac{\beta}{\sqrt{2}} I_3 , \quad (16)$$

where

$$I_n = \int_{u_1}^{u_2} du\, [V(u)]^{n/2} , \quad n = 1, 2, 3 . \quad (17)$$

Here we have used the relation $u_0' = \sigma\sqrt{2V(u_0)}$, $\sigma = \pm 1$. Therefore in the case of the ϕ^4 and sG models, we have

$$m_k = \tfrac{4}{3}\sqrt{2} - \tfrac{8}{45}\alpha\sigma - \tfrac{2}{35}\sqrt{2}\,\beta \quad (\phi^4 \text{ model}) ,$$

$$= 8 - \tfrac{4}{3}\pi\alpha\sigma - \tfrac{16}{3}\beta \quad (\text{sG model}) . \quad (18)$$

critical velocity is here only for local expansion (my old antikink) (if α<0 as for Toda)

3. Variational approach

In order to apply the variational method, it is important to notice that the solution of eq. (9) is actually the stationary point of the following functional,

$$E(u)=\int_{-\infty}^{\infty} dz\,[\tfrac{1}{2}\gamma^2u_z^2+\epsilon P(u_z)+V(u)]\,, \qquad (19)$$

because the variation of $E(u)$ is

$$\delta E(u)=\int_{-\infty}^{\infty} dz\,[-\gamma^2u_{zz}-\epsilon P''(u_z)u_{zz}+V'(u)]\delta u \qquad (20)$$

and $\delta E=0$ obviously leads to eq. (9).

The above observation will be the starting point of our variational method. Suppose that the main effect of the perturbation $\epsilon P(u_x)$ is to modify the kink shape, so that we will look for an approximate solution of eq. (9) in the form of the following ansatz (cf. ref. [13]),

$$u=\sigma\tanh(lz/\sqrt{2}) \quad (\phi^4 \text{ model}),$$
$$=4\tan^{-1}\exp(\sigma lz) \quad (\text{sG model}), \qquad (21)$$

where the parameter l^{-1} $(l>0)$ is the kink width and $\sigma=\pm1$ stands for the kink $(\sigma=+1)$ and the antikink $(\sigma=-1)$. Substituting eq. (21) into eq. (19) we obtain a function $E(l)$. The parameter l can be determined by looking for the minimum point of the function $E(l)$. For the cubic and quartic anharmonicities (15), the corresponding function $E(l)$ is

$$E(l)=\tfrac{1}{3}\sqrt{2}\,\gamma^2l+\tfrac{4}{45}\sigma\alpha l^2+\tfrac{2}{105}\sqrt{2}\,\beta l^3+\tfrac{1}{3}\sqrt{2}/l \quad (\phi^4 \text{ model}),$$
$$=4\gamma^2l+\tfrac{2}{3}\sigma\pi\alpha l^2+\tfrac{16}{9}\beta l^3+4/l \quad (\text{sG model}). \qquad (22)$$

The stationary point of $E(l)$ must satisfy the equation $dE/dl=0$, which yields

$$\gamma^2+\tfrac{4}{15}\sqrt{2}\,\sigma\alpha l+\tfrac{6}{35}\beta l^2-1/l^2=0 \quad (\phi^4 \text{ model}), \qquad (23a)$$

$$\gamma^2+\tfrac{1}{3}\sigma\alpha\pi l+\tfrac{4}{3}\beta l^2-1/l^2=0 \quad (\text{sG model}). \qquad (23b)$$

Note that if $\alpha=\beta=0$, eq. (23) will recover the exact relationship between γ and l, that is $l=1/\gamma$.

If α and β are small, it can be proved that both algebraic equations (23a) and (23b) have a solution which are the local minimum points of the function $E(l)$. The solutions are positive near $l=1/\gamma$. In principle, eqs. (23) may be solved by the Newton method. However, if the parameters α and β are sufficiently small, we can use the first-order approximation to obtain

$$l=(1-\tfrac{2}{15}\sqrt{2}\,\sigma\alpha/\gamma^3-\tfrac{3}{35}\beta/\gamma^4)/\gamma \quad (\phi^4 \text{ model}),$$
$$=(1-\tfrac{1}{6}\sigma\alpha\pi/\gamma^3-\tfrac{2}{3}\beta/\gamma^4)/\gamma \quad (\text{sG model}). \qquad (24)$$

This variational approach allows us to demonstrate some important effects due to anharmonic interactions. First, let us consider the ϕ^4 and sG chains with only cubic perturbation, then eqs. (23) reduce to

$$\gamma^2l^2+\tfrac{4}{15}\sqrt{2}\,\sigma\alpha l^3-1=0 \quad (\phi^4 \text{ model}),$$
$$\gamma^2l^2+\tfrac{1}{3}\pi\sigma\alpha l^3-1=0 \quad (\text{sG model}). \qquad (25)$$

If $\alpha\sigma<0$, it can be easily proved that the necessary conditions for eqs. (25) to have positive solutions are

$$\tfrac{25}{24}\gamma^6/\alpha^2\geqslant1 \quad (\phi^4 \text{ model}), \qquad (26)$$

$$\tfrac{4}{3}\gamma^6/\pi^2\alpha^2\geqslant1 \quad (\text{sG model}). \qquad (27)$$

Combining these two inequalities with eq. (7), we obtain the kink critical velocities in these two systems,

$$v_c^2=1-(\tfrac{24}{25}\alpha^2)^{1/3}\approx1-1.00\alpha^{2/3} \quad (\phi^4 \text{ model}), \qquad (28)$$

$$v_c^2=1-(\tfrac{3}{4}\pi^2\alpha^2)^{1/3}\approx1-1.95\alpha^{2/3} \quad (\text{sG model}). \qquad (29)$$

The phenomenon of the kink critical velocity due to anharmonic interatomic interactions was also discussed in refs. [1–12]. Here we may compare the results of the variational approach with the exact ones. Note that the first integral of eq. (9) is

$$\tfrac{1}{2}\gamma^2u_z^2+\tfrac{1}{3}\alpha u_z^3+\tfrac{1}{4}\beta u_z^4=V(u)\,. \qquad (30)$$

In case of $\alpha<0$ and $\beta=0$, the left hand side of eq. (30) as a function of u_z has a local maximum $\tfrac{1}{6}\gamma^6/\alpha^2$ at $u_z=-\gamma^2/\alpha$. In order that the kink solutions exist, the maximum value of the right hand side of eq. (30) must exceed that of the potential $V(u)$

for exponential (Toda) interaction, α < 0.
for compression (my old kink), σ = −1 here.
so (27, 29) is for local expansion (my old antikink)

(between the two equivalent ground states), which is $\frac{1}{4}$ for the ϕ^4, and 2 for the sG model (see ref. [12]). Therefore, we obtain the exact results for the critical velocities of the kink in these two systems:

$$v_c^2 = 1-(1.5\alpha^2)^{1/3} \approx 1-1.14\alpha^{2/3} \quad (\phi^4 \text{ model}), \tag{31}$$

$$v_c^2 = 1-(12\alpha^2)^{1/3} \approx 1-2.29\alpha^{2/3} \quad (\text{sG model}). \tag{32}$$

Comparing eqs. (28), (29) with eqs. (31), (32), we conclude that the variational method gives good estimations for the kink critical velocities.

Now let us use the approximate solutions (21) to calculate some physically important characteristics of the kinks. Substituting eq. (21) into the Hamiltonian (1) and using the interaction energy (4) and (15), we obtain the kink energy,

$$E_k = (\tfrac{1}{3}\sqrt{2}l)[1+l^2(1+v^2)] + \tfrac{4}{45}\alpha\sigma l^2 + \tfrac{2}{105}\sqrt{2}\beta l^3 \quad (\phi^4 \text{ model}),$$

$$= (4/l)[1+l^2(1+v^2)] + \tfrac{2}{3}\pi\alpha\sigma l^2 + \tfrac{16}{9}\beta l^3 \quad (\text{sG model}). \tag{33}$$

Analogously, the kink mass may be calculated as follows,

$$m_k = \int_{-\infty}^{\infty} \mathrm{d}z\, u_z^2|_{\gamma=1} = \tfrac{2}{3}\sqrt{2}\, l \quad (\phi^4 \text{ model}),$$

$$= 8l \quad (\text{sG model}), \tag{34}$$

where the parameter l is determined by eqs. (23). It is important to note that in the first-order approximation (24), the kink mass is *the same* as obtained by the perturbation approach (cf. eqs. (18), (24) and (34)). From these formulas we can see that, if the cubic anharmonicity parameter α is negative, then the kink profile is steeper than the antikink profile, in other words, the kink is narrower than the antikink. Meanwhile, the kink will have larger effective mass than the antikink, thus the kink–antikink symmetry is broken due to the anharmonicity. The difference in the masses may be calculated directly from eqs. (16) or (34), e.g., the first-order approximation result is

$$\frac{m_k - m_{\bar{k}}}{m_0} = \alpha \frac{2\sqrt{2}}{3} \frac{I_2}{I_1}, \tag{35}$$

where I_1 and I_2 are defined by eq. (17), and m_0 is the mass of the kink (k) and antikink ($\bar{\text{k}}$) in the unperturbed system.

The asymmetry may lead to important nontrivial physical phenomena in the study of mass transport along layers absorbed on crystal surfaces [10] and hydrogen-bonded chains [14]. For the latter systems, the asymmetry means that the mobilities of the positively and negatively charged defects (either ionic or bonding) are different.

As we have pointed out, for a given value of $\alpha < 0$, there exists a critical velocity for the kink. It means that there is a maximal energy for the kink in the system, which can be calculated by using eqs. (33), (28) and (29). On the other hand, it is easy to understand that there also exists a critical value for α, beyond which the kink will not exist. From (28) and (29) we can see that the critical values for α are ($v_c = 0$)

$$\alpha_c = -\sqrt{\tfrac{25}{24}} \quad (\phi^4 \text{ model}),$$

$$= -2/\pi\sqrt{3} \quad (\text{sG model}). \tag{36}$$

Substituting α_c into eqs. (25), we find that the critical value for l is $\sqrt{3}$ in both the ϕ^4 and sG system. Therefore from eq. (34) we may calculate the critical masses of the kink,

$$(m_k)_c = \tfrac{2}{3}\sqrt{6} \approx 1.633 \quad (\phi^4 \text{ model}),$$

$$= 8\sqrt{3} \approx 13.856 \quad (\text{sG model}). \tag{37}$$

Now let us check the above analytical results by numerical methods. We use a conservative scheme to discretize eq. (9) (see ref. [15]). The initial conditions are taken to be $(u(0), u_z(0)) = (0, u_1')$ from the ϕ^4 model, and $(u(0), u_z(0)) = (\pi, u_2')$ for the sG model, where u_1' and u_2' are determined by eq. (30). Due to symmetry we may carry out the calculations in the interval $(0, L)$ where L is taken to be 10. (The interval $(-10, 10)$ is large enough to contain a kink which is localized.) First, we integrate eq. (9) without perturbations ($\alpha = \beta = 0$). The numerical method gives very accurate results. For example, the kink mass calculated by the numerical method is accurate up to order 10^{-5} compared to the exact results. So we believe that the numerical integrator is absolutely reliable. Then we calculate the kink mass for different choices of the parameter α (β being equal to zero). The results are presented in figs. 1 and 2, from

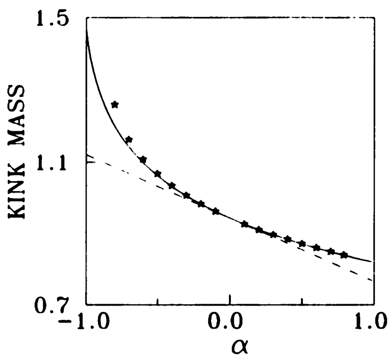

Fig. 1. Effective mass of the kink in the ϕ^4 model. The solid line is determined by the variational approach, the dashed line is a linear approximation (eq. (18)), the stars are the numerical results.

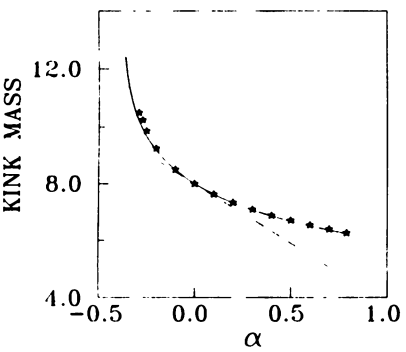

Fig. 2. The same as in fig. 1, but for the kink in the sine-Gordon model.

which we can see that the variational approach gives very good results. Furthermore, by numerical methods we find that the critical mass of the kink due to negative anharmonicity ($\alpha<0$) is about 1.3 and 11.0 in the ϕ^4 and sG models respectively, and these results agree with eqs. (37) estimated by the variational approach.

4. Conclusion

We have demonstrated that the variational approach may be applied to study the kink characteristics in the Klein–Gordon model including anharmonic interatomic interactions. It allows us to calculate the critical velocity and mass of the kink due to the anharmonicity with a good accuracy. Comparing the analytical results with numerical simulations for the ϕ^4 and sG models, we conclude that the variational approach gives much better results than the direct perturbation method.

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