PHYSICAL REVIEW E VOLUME 47, NUMBER 6 JUNE 1993

Asymptotic behavior of one-dimensional nonlinear discrete kink-bearing systems in the continuum limit: Problems of nonuniform convergence

S. Flach* and C. R. Willis
Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215
(Received 22 December 1992)

We study the validity of perturbational treatments of one-dimensional weakly discrete kink-bearing systems with the corresponding continuum model as the unperturbed state. We calculate the Peierls-Nabarro barrier height $\Delta_{\rm PN}$, the Peierls-Nabarro frequency $\omega_{\rm PN}$, and the deviation of the kink creation energy from the continuum case. In the case of the sine-Gordon system and the Φ^4 system, we find that the dressing (change of the continuum kink shape due to discreteness) contributes to the values of $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ through all orders of perturbation, thereby making the whole perturbation scheme irrelevant. In contrast, the double-quadratic model (where the whole necessary nonlinearity is "hidden" in one nonanalytic point) can be treated by the perturbation scheme without restrictions. The results found in this paper put general limitations on analytical approaches to nonlinear phenomena in discrete systems and demonstrate a deep inherent difference between corresponding discrete and continuum models.
PACS number(s): 03.20.+i ; 03.40.-t ; 63.20.Ry

I. INTRODUCTION

Solitary waves and solitons are a standard tool in understanding a large number of phenomena in condensed-matter physics such as dislocation kinetics, structural phase transitions, charge-density waves in polymer chains, flux quanta on Josephson-junction transmission lines, etc. [1,2]. In most cases the underlying structure of the system is discrete, i.e., we are confronted with a nonlinear lattice problem.

In order to find an approximate analytic description of the nonlinear excitations, one can consider the corresponding continuum model [3]. The discreteness effects can then be calculated in different kinds of perturbation approaches, treating the discreteness as a small perturbation [4–15]. Indeed typical models such as the discrete sine-Gordon (SG), Φ^4, etc. have a control parameter, which transforms the discrete system into the corresponding continuum one in a special limit, hereafter named as the *continuum limit*.

In the present paper we will consider one-kink properties in one-dimensional kink-bearing discrete systems. We will show that the mentioned perturbation approach in the continuum limit gives correct results for several properties such as the kink creation energy and mass. But surprisingly the perturbation approach *fails* to account for the height of the Peierls-Nabarro barrier $\Delta_{\rm PN}$ and frequency $\omega_{\rm PN}$, two of the essential properties of kinks in a discrete system in contrast to the continuum case. We will show that *all* terms in the perturbation series contribute in leading order to the values of $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ in the continuum limit. Thus we find a deep inherent difference between the discrete and continuum cases, making it impossible to connect them in an analytical way using the perturbation approach. This result puts general restrictions on analytical approaches to nonlinear phenomena in discrete systems.

The paper is organized as follows: in Sec. II we introduce the models and the kink solutions as well as their properties. In Sec. III we apply the usual perturbation scheme in the continuum limit. In Sec. IV we demonstrate that even in the lowest order of this perturbation approach a (solvable) difficulty appears. This difficulty is then the key of understanding why all orders of the perturbation scheme contribute to the $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ in leading order, thus making a perturbation ansatz irrelevant. In Sec. V we discuss our results and summarize the contents of the paper.

II. MODELS, KINK SOLUTIONS

We study a class of $d = 1$ dimensional discrete classical models given by the Hamiltonian

$$H = \sum_l [\tfrac{1}{2}P_l^2 + \tfrac{1}{2}C(Q_l - Q_{l-1})^2 + V(Q_l)] \quad . \qquad (1)$$

P_l and Q_l are canonically conjugated momentum and displacement of the lth particle, where l marks the number of the unit cell. C measures the interaction to the next-neighbor particles. All variables are dimensionless. The mass of the particles is equal to unity. The nonlinearity occurs in the "on-site" potential $V(x)$. In this paper we will discuss three different types of $V(x)$, (1) sine-Gordon (SG)

$$V(x) = V_{\rm SG}(x) = 1 - \cos(x) \quad , \qquad (2)$$

(2) Φ^4

$$V(x) = V_{\Phi^4}(x) = \tfrac{1}{4}(x^2 - 1)^2 \quad , \qquad (3)$$

(3) double quadratic (DQ)

$$V(x) = V_{\rm DQ}(x) = \tfrac{1}{2}(|x|-1)^2 \quad . \qquad (4)$$

All three examples are multiwell potentials leading to multiple degenerated ground states of the Hamiltonian (1). The SG case gives countable infinite degenerated ground states. In contrast, the Φ^4 and DQ potentials have only two degenerated ground states. The important difference between DQ on one side and Φ^4 and SG on the other side is that the whole nonlinearity of the DQ potential is located in the point $x=0$. We will see later that this simplification of a general multiwell potential has important consequences on the asymptotic behavior of the DQ system compared to cases (2) and (3). Let us also mention that the main mathematical difference between the Φ^4 on one side and the SG on the other side is that the former is not integrable in the continuum description, whereas the latter is. Thus we expect to have a representative set of different models.

The continuum-energy expression corresponding to the discrete Hamiltonian (1) is

$$H^c = \int dx \left[\frac{1}{2}\left(\frac{\partial Q}{\partial t}\right)^2 + \tfrac{1}{2}C\left(\frac{\partial Q}{\partial x}\right)^2 + V(Q)\right] \quad . \qquad (5)$$

The equation of motion for the field $Q(x,t)$ becomes

$$\frac{\partial^2 Q}{\partial t^2} - C\frac{\partial^2 Q}{\partial x^2} + \frac{\partial V}{\partial Q} = 0 \ . \qquad (6)$$

In this case the one-kink solutions $Q(x) = f^c(x)$ for (2)–(4) are known [16,17]:
(1) SG

$$f^c_{\rm SG}(x) = 4\arctan(e^{x/\sqrt{C}}) \quad , \qquad (7)$$

(2) Φ^4

$$f^c_{\Phi^4}(x) = \tanh\left(\frac{x}{\sqrt{2C}}\right) \quad , \qquad (8)$$

(3) DQ

$$f^c_{\rm DQ} = {\rm sgn}(x)[1-e^{-|x|/\sqrt{C}}] \quad . \qquad (9)$$

In the limit $C\to\infty$ the spatial variations of f^c in (7)–(9) become very slow, leading to the suggestion that the corresponding solution of the discrete lattice (1) with a fixed lattice spacing can be asymptotically described by the continuum kink shape $f^c(x)$. For the DQ case the corresponding discrete kink shape is known exactly [18]. Performing the limit $C\to\infty$ (continuum limit) indeed yields (9). For the SG case numerical simulations confirmed the mentioned connection of the discrete and continuum models [11]. Thus it becomes plausible to search for inherent discrete properties of a kink solution of (1) using the kink shape of the corresponding continuum model (5). Of course the deviations from the exact result will increase with decreasing C, but in the continuum limit those results should give the leading-order contribution to the properties under discussion. This approach indeed led to the understanding of the trapping of a kink in a discrete lattice. The trapping of the kink occurs due to the existence of a Peierls-Nabarro potential which is felt by the kink during the motion through the lattice [8]. The potential is periodic with a period equal to the lattice constant. The energy difference between a maximum and a minimum of the potential is the PN barrier ($\Delta_{\rm PN}$). If the kink is created with a too little kinetic energy, the kink is trapped between two maxima of the potential. For small amplitudes the center of mass of the kink should oscillate with a frequency $\omega_{\rm PN}$, the PN frequency. Including the fact of interaction between the kink and phonons (radiation) the scenario can be changed. But the existence of a well-defined $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ is still possible and meaningful [11].

To find the equation of motion of a kink in a lattice one has to introduce a new (time-dependent) coordinate—the position of the kink or center of mass $X(t)$ [19]. The kink manifests himself by a distortion of the lattice

$$Q_l(t) = f_l(X(t)) + q_l(t) \quad . \qquad (10)$$

$q_l(t)$ is the so-called dynamic dressing, i.e., these functions account for all lattice distortions not represented by the (still unknown) function f_l. Since the original N-particle system has a $2N$-dimensional phase space, the introduction of $X(t)$ and the canonically conjugated momentum $\Pi(t)$ increase the dimension by two. Thus one has to use two constraints reducing the (2N+2)-dimensional phase space to the original one [10]. These constraints can be chosen as

$$\sum_l f'_l(X) q_l = 0 \quad , \qquad (11)$$

$$\sum_l f'_l(X) p_l = 0 \quad , \qquad (12)$$

where a prime denotes differentiation with respect to the argument and p_l are the momenta canonically conjugated to q_l. This collective-coordinate method [19] leads to the following equation of motion for $X(t)$, neglecting the dynamic dressing at the end of the derivation [this step corresponds to an "adiabatic approximation"—we hold the kink center at a given X and let the system relax; then we change X to $(X+dX)$ and repeat the procedure, obtaining the X-dependent kink energy, and by differentiation the force] and thus the nongradient $\dot{X}$-dependent terms

$$\ddot{X} + \frac{1}{M(X)}\sum_l f_l(X) \left.\frac{\partial H}{\partial Q_l}\right|_{Q_l=f_l(X)} = 0 \quad , \qquad (13)$$

$$M(X) = \sum_l f'^2_l(X) \quad . \qquad (14)$$

The expression

$$U_{\rm PN}(X) = \sum_l f'_l(X) \left.\frac{\partial H}{\partial Q_l}\right|_{Q_l=f_l(X)} \qquad (15)$$

is the Peierls-Nabarro potential. This potential is felt by the moving kink according to (13). The creation energy of a kink at position X is given by

$$E_K(X) = H|_{Q_l=f_l(X)} \quad . \qquad (16)$$

We can separate $U_{\rm PN}$ from $E_K(X)$,

$$E_K(X) = E_K + U_{\rm PN}(X) \quad . \tag{17}$$

In the corresponding continuum model (5) the creation energy is given by

$$E_K^c = H^c(Q(x) = f^c(x)) \quad . \tag{18}$$

For our cases under consideration we find (1) SG

$$E_K^c = 8\sqrt{C} \quad , \tag{19}$$

(2) Φ^4

$$E_K^c = \tfrac{2}{3}\sqrt{2C} \quad , \tag{20}$$

(3) DQ

$$E_K^c = \sqrt{C} \quad . \tag{21}$$

The energy deviation

$$U_0 = E_K - E_K^c \tag{22}$$

measures the difference between the mean kink creation energy on the lattice compared to the corresponding continuum value. As we will see, $\max[|U_{\rm PN}(X)|]/|U_0|$ will decrease exponentially with increasing C in the continuum limit, thus making it reasonable to account for two different properties: U_0 as the mean deviation of the creation energy from the continuum value and $U_{\rm PN}(X)$ as an (exponentially) small overlayed X-dependent potential. Through the simple relation

$$E_K^c = M^c C \quad , \tag{23}$$

one finds the corresponding continuum mass of a kink M^c. Note that in the continuum case E_K^c and M^c do not depend on the position of the center of mass of the kink X in contrast to the discrete case (14) and (16).

III. STATIC PERTURBATION APPROACH

Since the exact kink shape of the continuum model (5) is usually known [for a given $V(x)$] it seems to be meaningful to apply a perturbation scheme to the discrete system (1) where the unperturbed solution is that of the corresponding continuum model. Both models seem to be connected in the limit $C \to \infty$, consequently the perturbation scheme is expected to be reasonable at least in this limit. However, results of several numerical investigations [8,20] might question the validity of the above statement. But no serious attempt was done in order to study this problem. We will return to these results at the end of this section.

Let us follow now the main steps of the perturbation scheme as developed in [10] and [11]. Although there are slight differences in perturbation schemes of other authors, these differences will not affect the solution of the problem we are dealing with. In that sense they are equivalent.

First we introduce the *static* dressing q_l^s, which measures the difference between the static discrete kink profile f and the continuum one f^c,

$$f_l(X) = f_l^c(X) + q_l^s(X) \quad . \tag{24}$$

$f_l^c(X)$ means $f^c(l-X)$ [cf. (7)–(9)]. Using the equation of motion

$$\ddot{Q}_l = -\frac{\partial H}{\partial Q_l} \quad , \tag{25}$$

the Lagrangian multiplier term

$$\lambda(X)\sum_l f_l^{c\prime}(X) q_l^s(X) \quad , \tag{26}$$

which is added to the original Hamiltonian in order to hold the kink at an arbitrary X, and setting the left side of (25) equal to zero, we then obtain

$$(-f_{l+1}^c + 2f_l^c - f_{l-1}^c) + (-q_{l+1}^s + 2q_l^s - q_{l-1}^s) + \left.\frac{\partial V}{\partial Q_l}\right|_{Q_l = f_l^c + q_l^s} + \lambda f_l^{c\prime} = 0 \quad . \tag{27}$$

Note that we have suppressed the notation of the X dependence in (27) for the sake of simplicity. Equation (27) is a nonlinear equation for $q_l^s(X)$ and $\lambda(X)$. In [11] (27) was linearized with respect to q_l^s thus calculating the first-order static dressing. It is not of relevance here to procceed in the same way. We only note the important result that by using the expansion

$$-f_{l+1}^c(X) + 2f_l^c(X) - f_{l-1}^c(X) = -2\sum_{m=1}^{\infty} \frac{1}{(2m)!} f_l^{c(2m)}(X) \tag{28}$$

[where the index $(2m)$ means the $(2m)$th derivative with respect to the argument] it follows from (27) that q_l^s is a functional of the set of functions $\{f_l^{c(m)}(X)\}_{m=0,1,\ldots}$. Now let us start the perturbation scheme with the zero-order step: we neglect the static dressing completely, thus assuming

$$f_l^0(X) = f_l^c(X) \quad . \tag{29}$$

Inserting (29) into (13) and using the equation of motion for $f_l^c(X)$ (6) we find [10]

$$\ddot{X} = \frac{2C}{M(X)} \sum_l \sum_{m=2}^{\infty} \frac{1}{(2m)!} f_l^{c\prime}(X) f_l^{c(2m)}(X) \,. \tag{30}$$

Since the double sum on the right-hand-side (rhs) of (29) is a function periodic in X with period of a lattice spacing, we can represent it in a Fourier series expansion,

$$\sum_l \frac{2C}{(2m)!} f_l^{c\prime}(X) f_l^{c(2m)} = \sum_{n=1}^{\infty} B_{nm} \sin(2\pi n X) dX \;, \tag{31}$$

$$B_{nm} = -\frac{4C}{(2m)!}\int_{-\infty}^{+\infty} f^{c\prime}(x) f^{c^{(2m)}}(x)\cdot \sin(2\pi n x)dx$$
$$= \frac{2C}{\pi n (2m)!}\int_{-\infty}^{+\infty}[f^{c^{(2)}}(x)f^{c^{(2m)}}(x) + f^{c\prime}(x)\cdot f^{c^{(2m+1)}}(x)] \times \cos(2\pi n x)dx \ . \quad (32)$$

It follows

$$\ddot{X} = \frac{1}{M(X)}\sum_{n=1}^{\infty} B_n \sin(2\pi n X)\ , \quad (33)$$

$$B_n = \sum_{m=2}^{\infty} B_{nm}\ . \quad (34)$$

Thus we find an X-dependent $U_{\rm PN}$ [cf. (15)] even in the zero-order perturbation approach. If $f_l^c(X)$ is statically dressed there will be an additional X-dependent contribution to $U_{\rm PN}$. However, since the dressing contribution is of higher order within the perturbation approach, it would seem reasonable to assume the dressing is negligible in the continuum limit. Therefore we define assumption (1) as follows: we assume Eqs. (33) and (34) give the correct result for $U_{\rm PN}$ (and thus for $\Delta_{\rm PN}$ and $\omega_{\rm PN}$) in leading order for $C \to \infty$.

In the zero-order perturbation approach [assumption (1)] we obtain for $U_{\rm PN}$

$$U_{\rm PN}(X) = \sum_{n=1}^{\infty}\frac{B_n}{2\pi n}\cos(2\pi n X) \ . \quad (35)$$

If $(B_{n+1}/B_n)|_{C\to\infty} \to 0$, we can state that the periodic function $U_{\rm PN}(X)$ has minima at $X_{\rm min} = \frac{1}{2} \pm k$ and maxima at $X_{\rm max} = \pm k$ with $k = 0, \pm 1, \pm 2, \ldots$. Then it follows for the Peierls-Nabarro barrier height $\Delta_{\rm PN}$:

$$\Delta_{\rm PN} = \frac{1}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}B_{2n+1} \ , \quad (36)$$

i.e., only the odd n in (35) contribute to $\Delta_{\rm PN}$. From (33) it follows that for small-amplitude oscillations of the kink around a minimum of the $\Delta_{\rm PN}$ we find a solution $X(t) \sim \cos(\omega_{\rm PN} t + \alpha)$, where $\omega_{\rm PN}$ is given by

$$\omega_{\rm PN}^2 = \frac{1}{M(\frac{1}{2})}\sum_{n=1}^{\infty}(-1)^{n+1} 2\pi n B_n \ . \quad (37)$$

Finally we give the relations for the kink mass and energy correction U_0 in the zero-order approximation. The mass (14) is given by

$$M(X) = \tfrac{1}{2}A_0 + \sum_{n=1}^{\infty} A_n \cos(2\pi n X)\ , \quad (38)$$

$$A_n = 2\int_{-\infty}^{+\infty} f^{c\prime 2}(x)\cos(2\pi n x)dx\ . \quad (39)$$

The energy correction yields

$$U_0 = \tfrac{1}{2}C\sum_{m,m'=1}^{\infty}\frac{1-\delta_{1,m}\delta_{1,m'}}{m!m'!} \times \int_{-\infty}^{+\infty} f^{c^{(m)}}(x) f^{c^{(m')}}(x)dx\ . \quad (40)$$

Now we come to assumption (2). Since all continuum kink shapes are functions of the reduced distance variable $\tilde{x} = x/\sqrt{C}$ [cf. (7)–(9)] one finds

$$f^c(x/\sqrt{C}) = g(\tilde{x}) \ , \quad (41)$$
$$f^{c^{(m)}}(x) = C^{-m/2} g^{(m)}(z)|_{z=x/\sqrt{C}} \ . \quad (42)$$

Therefore we define assumption (2) as follows: requiring assumption (1) we assume in all expressions, where sums over derivatives of $f^c(x)$ of different order appear, to keep only the term(s) with the lowest-order derivative with respect to powers of $C^{-1/2}$.

Let us discuss the validity of the described two assumptions in the light of previous work. On one side the static dressing for the SG case indeed becomes small in the continuum limit (compared to the continuum shape) [11]. On the other side Combs and Yip (cf. Fig. 9 in [8]) found in the Φ^4 case an indication of nonconvergence between the zeroth-order result [assumption (1)] and the exact one for $U_{\rm PN}$, although they vary the parameter C only between 0.1 and 1. Boesch and Willis stress in [20] a possible failure of assumption (2), i.e., that higher-order derivative terms have to be taken into account to find the zeroth-order result for $\Delta_{\rm PN}$ and $\omega_{\rm PN}$. This fact was also mentioned by Ishimori and Munakata who used a different perturbation method due to McLaughlin and Scott in the SG case [7]. Thus the question arises whether the above described assumptions are valid or not.

In Sec. IV we will show that assumption (2) is correct for U_0, whereas it is incorrect for $\Delta_{\rm PN}$ and $\omega_{\rm PN}$. We will see that it is still possible to find the correct asymptotic behavior under assumption (1).

IV. THE ASYMPTOTIC BEHAVIOR

A. Some useful relations

In Sec. III we dealt with the real part of quantities of the following type:

$$I_{mk}(\omega) = \int_{-\infty}^{+\infty} f^{c^{(m)}}(x) f^{c^{(k)}}(x) e^{i\omega x}dx\ , \quad (43)$$

where ω could be finite or zero. With (41) and (42) it follows:

$$I_{mk}(\omega) = C^{-\frac{1}{2}(m+k-1)}\tilde{I}_{mk}(\tilde{\omega})|_{\tilde{\omega}=\omega\sqrt{C}}\ , \quad (44)$$

$$\tilde{I}_{mk}(\omega) = \int_{-\infty}^{+\infty} g^{(m)}(x) g^{(k)}(x) e^{i\omega x}dx\ . \quad (45)$$

Viewing (45) as a Fourier transformation and introducing

$$g_m(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} g^{(m)}(x)e^{i\omega x}dx \quad (46)$$

and using $g^{(m)}(x \to \pm\infty) = 0$ for $m \geq 1$, one finds with $g_n(\omega) = (-i\omega)^{n-1} g_1(\omega)$,

$$\tilde{I}_{mk}(\omega) = (-i)^{m+k-2} \int_{-\infty}^{+\infty} \nu^{m-1}(\omega-\nu)^{k-1} \times g_1(\nu) g_1(\omega-\nu) d\nu \,. \quad (47)$$

It follows immediately that $\tilde{I}_{mk}(\omega = 0)$ is independent of C and

$$I_{mk}(0) \sim C^{-\frac{1}{2}(m+k-1)} \quad . \quad (48)$$

Assumption (2) is thus indeed correct for terms with $n = 0$ in (38) and (40). However, the terms with $n \neq 0$ in (32) and (39) are more complicated. If we discuss continuum kink shapes with the properties

$$g_1(\omega) = g_1(-\omega), \;\; g_1(\omega \to \infty) = R(\omega) e^{-\alpha\omega} \;, \quad (49)$$

where $R(\omega)$ is some rational function of ω and α is positive, we find

$$I_{mk}(\omega \to \infty) \approx (-i\omega)^{m+k-2} e^{-\alpha\omega} \xi(\omega) \,, \quad (50)$$

$$\xi(\omega) = \int_{-\infty}^{+\infty} g_1(\nu) g_1(\omega-\nu) d\nu \,. \quad (51)$$

Then it follows

$$I_{mk}(\omega)|_{C\to\infty} = \frac{1}{\sqrt{C}} e^{-\alpha\sqrt{C}\omega} (-i\omega)^{m+k-2} \xi(\omega) \,, \quad (52)$$

i.e., the C dependence of I_{mk} becomes independent of m and k in the continuum limit. But this result would immediately call into question assumption (2), as we will show in the following subsections.

B. Φ^4 case

For $f^{c\prime}(x)$ we have

$$f^{c\prime}(x) = \frac{1}{2C} \text{sech}^2 \frac{x}{\sqrt{2C}} \quad . \quad (53)$$

Then it follows

$$g'(x) = \text{sech}^2(x) \quad , \quad (54)$$

$$g^{(2)^2} = 4(g'^2 - g'^3) \quad , \quad (55)$$

$$g^{(3)} = 4g' - 6g'^2 \quad , \quad (56)$$

$$g^{(2m+1)} = \cdots g' + \cdots g'^2 + \cdots + D_{2m+1} g'^{m+1} \quad , \quad (57)$$

$$D_{2m+1} = (-1)^m (2m+1)! \quad . \quad (58)$$

Thus in (32) we are dealing with a series of integrals over powers of $\text{sech}^2(x/\sqrt{C})$ multiplied by a $\cos(2\pi n x)$ factor. Such integrals can be found in the tables in [21]

$$\int_0^\infty \text{sech}^{2m}\left(\frac{x}{\sqrt{2C}}\right) \cos(2\pi n x) dx = \frac{4^{n-1}\pi^2 2nC}{(2m-1)! \sinh(\pi^2 n\sqrt{2C})} \prod_{k=1}^{m-1} (2\pi^2 n^2 C + k^2) \,. \quad (59)$$

The highest-order power of sech^2 gives the leading-order contribution in the continuum limit. Consequently we find for B_{nm} in the continuum limit

$$B_{nm} = \frac{(-1)^m}{(2m+2)!} \pi^{2m+3} n^{2m+2} 2^{2m+5} \frac{C^2}{\sinh(n\pi^2\sqrt{2C})} \,. \quad (60)$$

As expected in Sec. IV A, the asymptotic C dependence of B_{nm} is independent of m in the continuum limit. By summation over all m we obtain

$$B_n = 4^2 \pi^3 n^2 (\tfrac{1}{3}\pi^2 n^2 - 1) \frac{C^2}{\sinh(n\pi^2\sqrt{2C})} \,. \quad (61)$$

A test of the order of error obtained within assumption (2) in comparison to assumption (1) can be given calculating

$$\left.\frac{B_{nm}}{B_n}\right|_{m=2} = \tfrac{2}{1}5(\pi n)^4 \frac{1}{(\pi n)^2 - 3} \,. \quad (62)$$

E.g., for $n = 1$ (62) yields 1.89. To demonstrate the validity of our result, we calculate the asymptotic Peierls-Nabarro barrier height $\Delta_{\rm PN}^{\rm as}(C)$ from (36) with (61) and compare it with the numerical value, $\Delta_{\rm PN}^{\rm 0\,order}(C)$, obtained within assumption (1) (i.e., within the zeroth order of perturbation) by shifting the continuum kink shape through the lattice in Fig. 1(a) (log-log plot) and Fig. 1(b) (semilogarithmic plot). In Fig. 2 we plot the ratio $\Delta_{\rm PN}^{\rm as}/\Delta_{\rm PN}^{\rm 0\,order}$ as a function of C. We see that for $C \geq 5$ the deviation of $\Delta_{\rm PN}^{\rm as}$ compared to $\Delta_{\rm PN}^{\rm 0\,order}$ is less then 1%. Remember that assumption (2) would lead to a 89% error [for $C \geq 4$ only the $n = 1$ term (B_1) gives the leading-order contribution due to the sinh in the denominator in (61)], cf. (62).

Now let us return to assumption (1). As we have seen in Sec. III, the static dressing is a functional of the derivatives of $f^c(x)$. Let us use the result of the first-order calculation of q^s from [11]. Then we assume that we can retain in all equations only the linear term in q^s. Due to the functional dependence on powers of $\text{sech}^2(x/\sqrt{C})$, we find after integration over the corresponding terms in (32), that the first-order dressing correction yields the same asymptotic dependence on C as the zero-order result terms. Thus the first-order correction has to be taken into account in the continuum limit calculating the values of $\Delta_{\rm PN}$ and $\omega_{\rm PN}$. If we now study the higher-order terms in q^s in the expressions of $\Delta_{\rm PN}$ (or $\omega_{\rm PN}$) we, however, again find that they also contribute to a leading-order result. We are confronted with the somewhat confusing result that *all* orders of perturbation contribute to the leading-order result for Δ_{PN} and ω_{PN}. The solution of the problem is simply that assumption (1), i.e., the application of a perturbation scheme with the continuum model as the unperturbed state, is false. Thus we arrive at a very nontrivial point—there is no simple connection between discrete and corresponding continuum systems in the continuum limit. To demonstrate that our zero-order result indeed fails to account for the whole leading-order result, we calculate numerically the *exact* Peierls-Nabarro barrier height Δ_{PN}^{exact} (as described in [20], i.e., via minimization of the energy functional under the constraint $X = 0.5$ and $X = 0$, respectively; obtaining the exact kink shape we calculate the energy difference of both solutions) and compare it with our old results Δ_{PN}^{as} and $\Delta_{PN}^{0\,order}$ in Figs. 3(a) and 3(b). The plots indicate that the zero-order perturbation result does not converge to the exact one in the continuum limit. In Fig. 4 we plot $\Delta_{PN}^{0\,order}/\Delta_{PN}^{exact}$ vs $\log_{10} C$. We see that the ratio converges to a value about 0.2 for large C. Thus we lost 80% of the true result neglecting the static dressing. Assumption (1) therefore becomes false, and the whole perturbation approach fails in accounting for the Δ_{PN} and ω_{PN}.

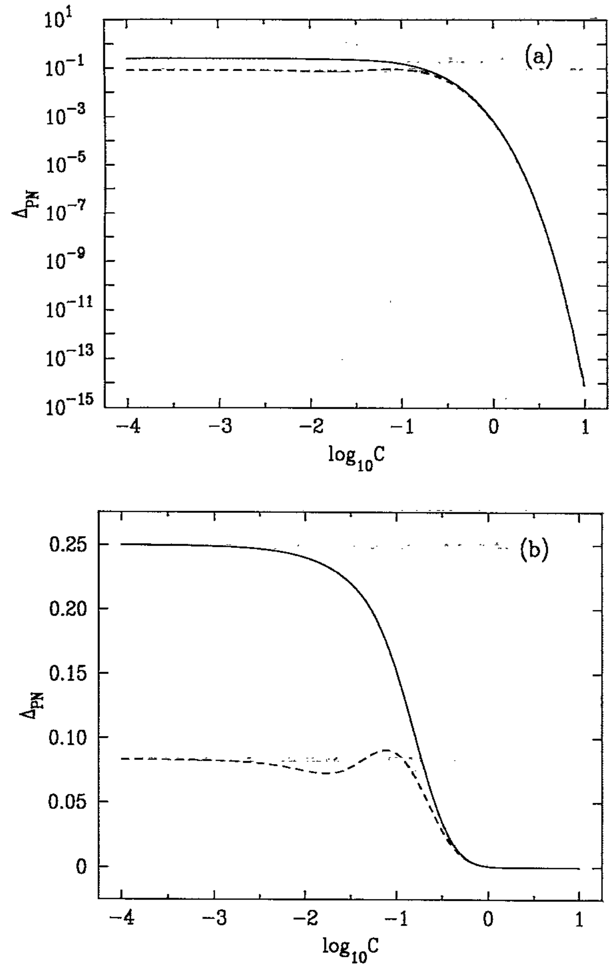

FIG. 1. Δ_{PN} vs $\log_{10}$C for Φ^4. Solid line, zero-order perturbation result $\Delta_{PN}^{0\,order}$, dashed line, asymptotic leading-order result Δ_{PN}^{as} (36) and (61); (a)Δ_{PN} on a logarithmic scale and (b)Δ_{PN} on a linear scale.

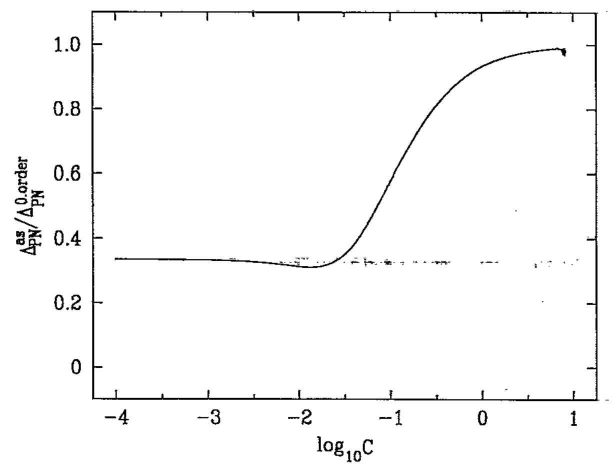

FIG. 2. Ratio of the asymptotic leading-order result for the Δ_{PN} over the correct zero-order perturbation result for Φ^4 $\Delta_{PN}^{as}/\Delta_{PN}^{0\,order}$ vs $\log_{10}$C.

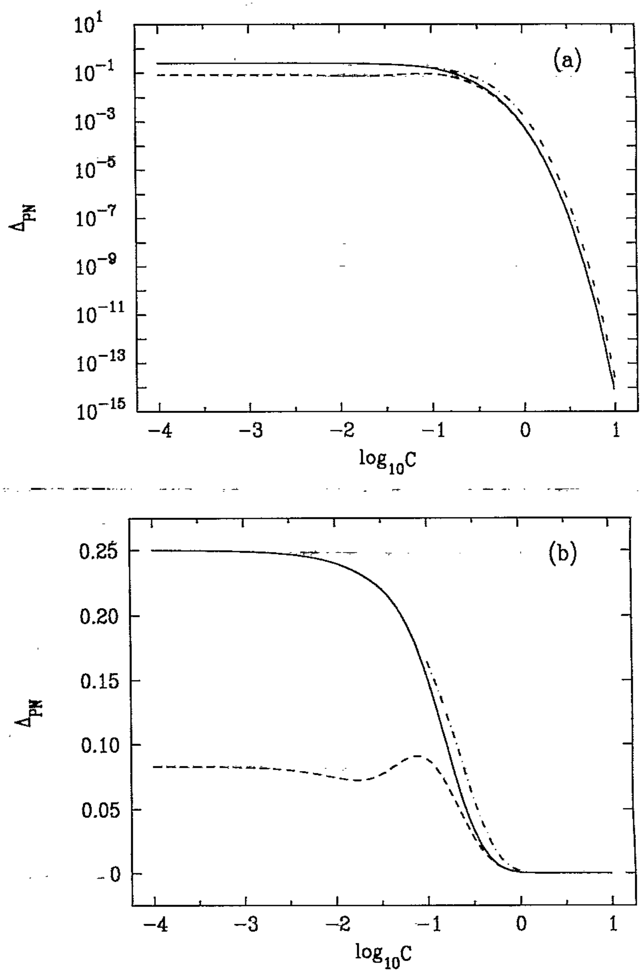

FIG. 3. Same as Fig. 1 but with the additional exact Δ_{PN} Δ_{PN}^{exact} (dashed-dotted line) for Φ^4.

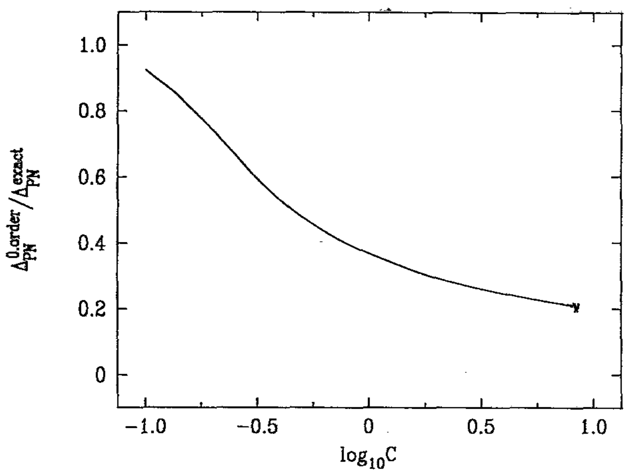

FIG. 4. Ratio of the exact $\Delta_{\rm PN}$ over the zero-order perturbation result $\Delta_{\rm PN}^{\rm exact}/\Delta_{\rm PN}^{0\ \rm order}$ vs $\log_{10}$C for Φ^4.

Finally we show in Fig. 5 the energy correction U_0 in zeroth order [i.e., under assumptions (1) and (2), keeping only the lowest terms (m,k)=(1,3),(3,1),(2,2) in (40)] compared to the exact solution. We find excellent agreement for $C \geq 1$. Consequently properties like the energy correction and also the mass indeed can be calculated using the perturbation scheme. We find nonuniform convergence in the sense that, depending on the properties one has to calculate, the described perturbation approach fails or not.

C. Sine-Gordon case

Here we have

$$g' = \mathrm{sech}(x) \ , \tag{63}$$

$$g^{(2)^2} = g'^2 - g'^4 \ , \tag{64}$$

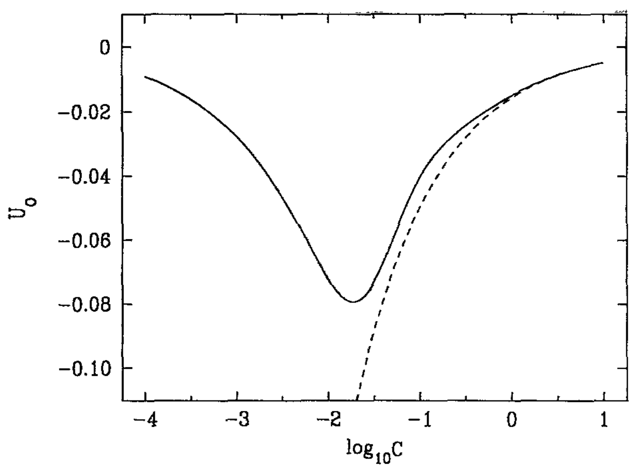

FIG. 5. U_0 vs $\log_{10}$C for Φ^4. Solid line, exact result; dashed line, leading-order perturbation result [assumptions (1) and (2)].

$$g^{(3)} = g' - 2g'^3 \ , \tag{65}$$

$$g^{(2m+1)} = g' + \cdots g'^3 + \cdots + D_{2m+1} g'^{2m+1} \ , \tag{66}$$

$$D_{2m+1} = (-1)^m (2m)! \ . \tag{67}$$

Keeping only the highest powers of sech (cf. Sec. IV B), we find in the continuum limit

$$B_{nm} = 2^{2m+4}(-1)^m n^{2m} \pi^{2m+1} \left(1 + \frac{1}{2m}\right) \times \frac{C}{(2m+1)! \sinh(n\pi^2\sqrt{C})} \ . \tag{68}$$

Again the asymptotic C dependence in the continuum limit is independent of m, leading to the result

$$B_n = \frac{C}{\sinh(n\pi^2\sqrt{C})} \left[2^4\pi[\tfrac{2}{3}(n\pi)^2 - 1] + \sum_{m=2}^{\infty} \frac{1}{2m} \tilde{B}_{nm} \right] \ , \tag{69}$$

$$\tilde{B}_{nm} = (-1)^m \frac{2^{2m+4}\ ^{2m}}{(2m+1)!} \pi^{2m+1} \ . \tag{70}$$

Calculating B_{12}/B_1 yields a 118% error of the assumption (2) compared with the correct zero-order result. It is interesting to note here that Ishimori and Munakata [7] found through a different perturbation approach the same value for B_1. In Figs. 6(a) and 6(b) we plot the asymptotic result $\Delta_{\rm PN}^{\rm as}$ from (36) and (69) and the correct numerical value (zero-order perturbation result) $\Delta_{\rm PN}^{0\ \rm order}$ vs C [the asymptotic result could not be calculated at low C because of convergence problems of the sum on the rhs of (69)]. The ratio of both values is given in Fig. 7 as a function of C, indicating a less than 1% error for $C > 1$. Remember that assumption (2) would lead to a 118% error. Thus we again find (cf. the discussion in Sec. IV B) that the static dressing will contribute to the leading-order result of $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ through all orders of perturbation. To show that we calculate numerically the *exact* Peierls-Nabarro barrier height $\Delta_{\rm PN}^{\rm exact}$ and compare it with the zero-order perturbation result in Figs. 8(a) and 8(b). In Fig. 9 we plot the ratio of the two values versus C. We see that the ratio converges to a value about 0.4 for large C. Thus we lost 60% neglecting the static dressing.

As in the Φ^4 case we calculate U_0 in zeroth-order perturbation and compare it with the exact value in Fig. 10. Again we find excellent agreement for $C > 1$.

D. DQ case

In the case of the DQ on-site potential (4) we cannot adopt the whole method of Sec. III. The reason is that (28) does not hold because of the nonanalytic behavior of $V(x)$ at $x = 0$. Thus the resulting $U_{\rm PN}$ is also pointwise nonanalytic (at its maxima, cf. [18]). Nevertheless it is not difficult to rewrite (28) in an appropriate manner. The main point is that, except for some additional

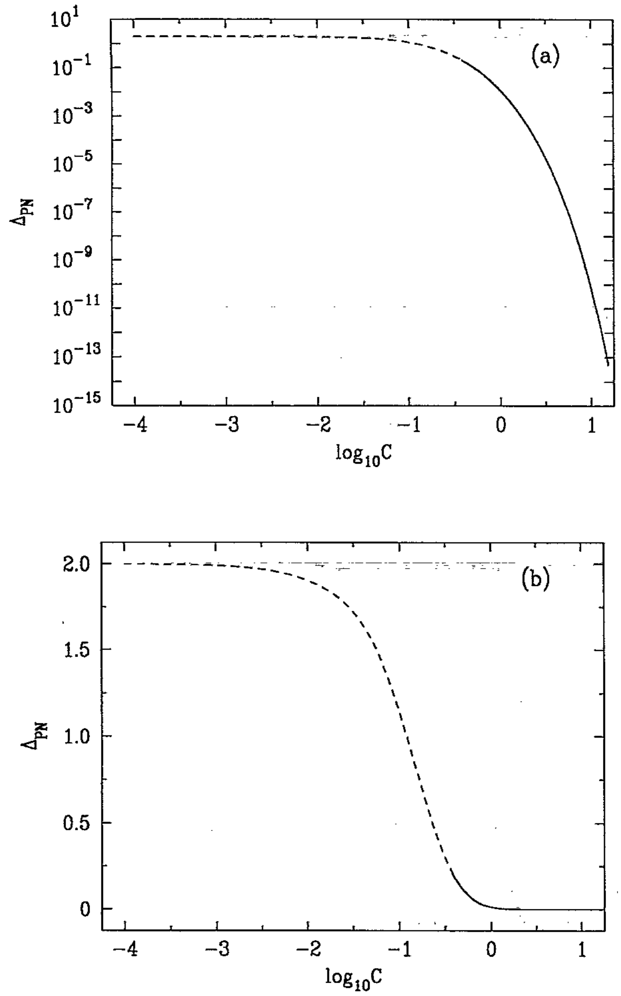

FIG. 6. Same as Fig. 1 but for SG. Dashed line, zero-order perturbation result $\Delta_{PN}^{0\,\mathrm{order}}$; solid line, asymptotic leading-order result Δ_{PN}^{as} (36),(69) and (70).

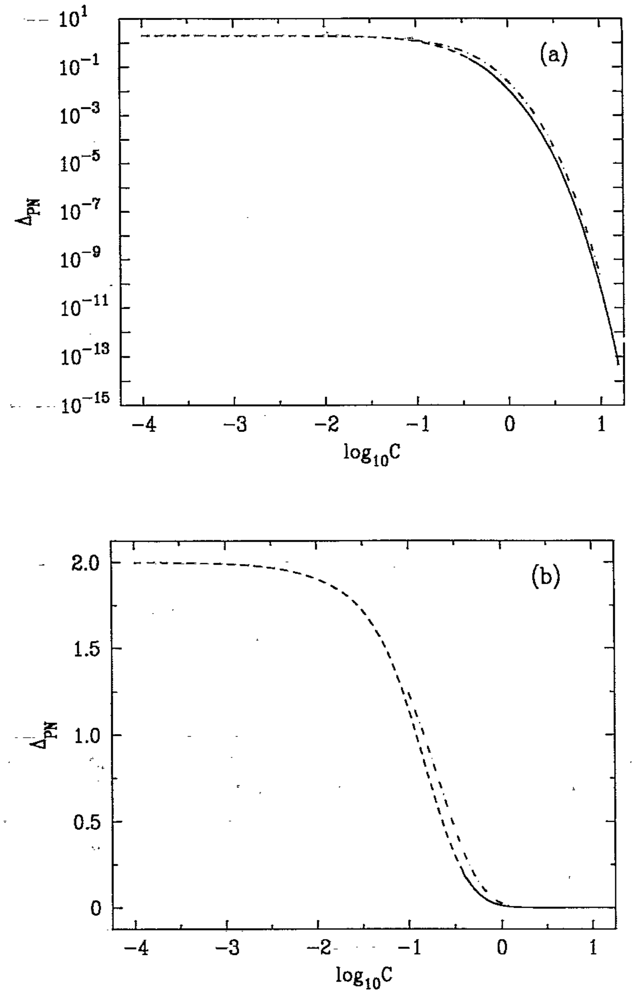

FIG. 8. Same as in Fig. 3 but for SG. Solid line, asymptotic leading-order result Δ_{PN}^{as}; dashed line, zero-order perturbation result $\Delta_{PN}^{0\,\mathrm{order}}$; dashed-dotted line, exact result Δ_{PN}^{exact}.

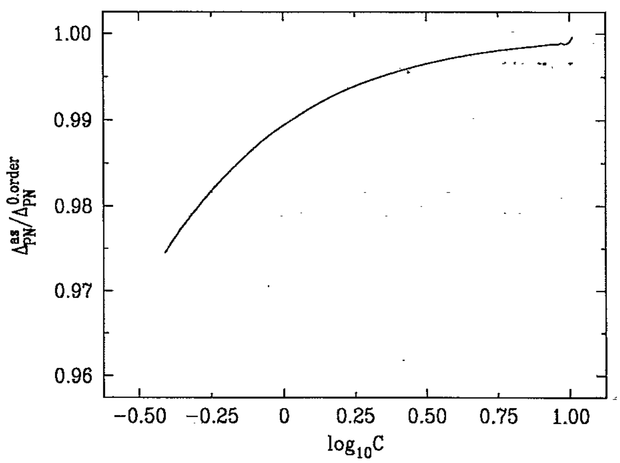

FIG. 7. Same as in Fig. 2 but for SG.

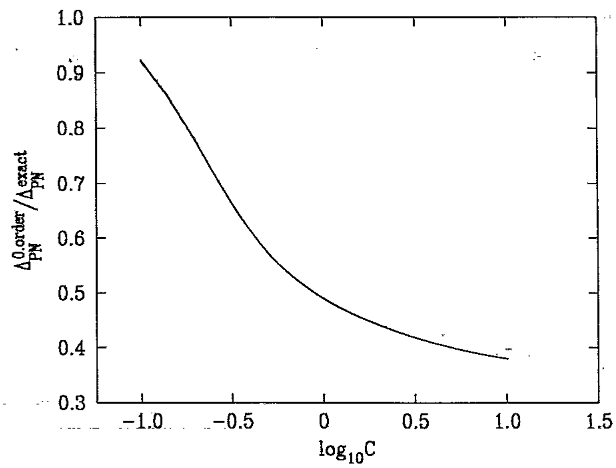

FIG. 9. Same as in Fig. 4 but for SG.

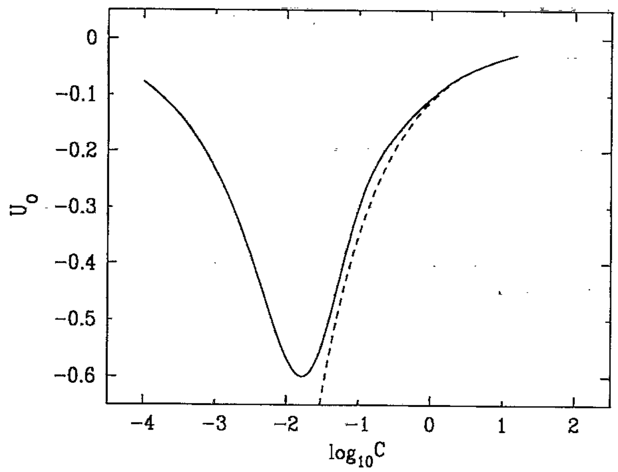

FIG. 10. Same as in Fig. 5 but for SG.

$e^{-x/\sqrt{C}}$ terms, we again replace the finite difference [left-hand-side (lhs) of (28)] by a sum over derivatives of (4). But it follows immediately from (4) that

$$|f_{\rm DQ}^{c(m+1)}(x)| = C^{-m/2}|f_{\rm DQ}^{c'}(x)| \ . \qquad (71)$$

This relation is different from the corresponding relations for the Φ^4 [(53)–(58)] and SG [(63)–(67)] cases. There we had instead of $f^{c'}(x)$ on the rhs of (71) a series of powers of $f^{c'}(x)$. It is easy to see that the additional summation over index l now causes the leading-order contribution for $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ in the DQ case to come from the lowest derivatives of $f_{\rm DQ}^{c}$. Thus assumption (2) becomes true, and with it also assumption (1), since the dressing will appear only in a higher order of powers of $C^{-1/2}$.

V. DISCUSSION

We have shown that the perturbation ansatz for the (weak) discrete model (1) with the continuum model (5) as the unperturbed state leads to the correct asymptotic result for the energy deviation U_0, but fails to account for the $\Delta_{\rm PN}$ and $\omega_{\rm PN}$. This result was already indicated in [8] for the Φ^4 case and in [20] for the SG case. The reason for the nonuniform convergence seems to be the interplay between discreteness and nonlinearity, since the DQ case [where the whole nonlinearity of the potential $V(x)$ is hidden in one point] behaves in the originally expected manner, i.e., the perturbation scheme is applicable without restrictions. It is interesting to note that the nonuniform convergence appears in the (integrable in the continuum) SG case as well as in the (nonintegrable in the continuum) Φ^4 case. Thus, indeed, the DQ case seems to be the atypical case with respect to the kink properties (as mentioned in [22,18]).

We want to stress a subtle point in the derivation of the asymptotic leading-order formula for B_{nm} in Sec. IV. If one considers the integral in (IV B) for a fixed m and lets C go to infinity, then the determination of the leading-order behavior (in C) causes no difficulty. However, what is needed is a fixed C in (32), whereas m in (IV B) has to be varied from 2 to infinity. It immediately becomes clear that there exists an upper (C-dependent) boundary for m, such that for larger m the leading-order C dependence of the integral on the lhs of (IV B) will become different. However, if C is large enough, that boundary for m will be also large enough, and the factorial in the denominator of the rhs of (IV B) will suppress the whole expression (compared to the lower terms in m which contribute in the sum over B_{nm}). Thus we are making an error in a part of the leading-order result, which is of zero weight.

Our results deal only with $\Delta_{\rm PN}$. The reader might ask whether the importance of the dressing comes from the differences of the dressing function if the kink center of mass is between two lattice sites or on a lattice site. If so, one could imagine that $\omega_{\rm PN}$ could be still calculated within the perturbation approach. The problem can be solved by stating that the functional C dependence of B_n is still correct (only the prefactor is wrong) as obtained from the perturbation approach for the SG and Φ^4 cases. Thus $U_{\rm PN}$ in the continuum limit is a cosine function, and the $\omega_{\rm PN}$ is connected through the strength B_1 with the $\Delta_{\rm PN}$. Then there is no doubt that the dressing will also contribute in leading order to the value of the $\omega_{\rm PN}$. We tested this conclusion by calculating the exact $\omega_{\rm PN}$ from the diagonalization procedure as, e.g., described in [20], and we found the same deviations from the perturbation result as for the $\Delta_{\rm PN}$. Consequently the "local" dressing gives contributions to the leading-order results for the $\Delta_{\rm PN}$ and $\omega_{\rm PN}$.

A mathematical indication of the nonuniform convergence found for models (1) with differentiable potentials $V(x)$ is given in (47). However, this might not be the only case where the nonuniform convergence holds. But still (47) can be used to test whether other suggested kink-bearing models [6,23,24] also exhibit nonuniform convergence, which would question the applicability of perturbation calculations.

The present paper also raises the question of the validity of the perturbation approach applied to other properties of kinks, such as kink-phonon interaction (Φ^4 [4]), phonon radiation (SG [7]), kink diffusion (Φ^4 [8]), as well as problems of the statistical-mechanics description (SG [13]) and kink properties under the presence of long-range interaction potentials (Φ^4 [14]).

It is legitimate to pose the question whether the presented results are a consequence of the particular choosen perturbation scheme or not. The answer is no, since we have verified numerically (Figs. 4 and 9) the main result, namely that the contribution of the static dressing to the leading-order C dependence of the $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ in the continuum limit takes place and is independent on the perturbation scheme. Moreover, the perturbation method applied in the present work is used to show the reasons for the main result of nonuniform convergence. That the perturbation method can be successfully applied to several quantities is also shown in [11], where the static dressing is calculated in first-order perturbation theory and gives excellent agreement with numerical solutions. However, as we have shown, several quantities like the $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ are defined through integrals over the corresponding terms. Because of the subtle behavior of these integrals we find the surprising fact that terms negligible in the calculation of the integrands cannot be neglected in evaluating the integrals.

An interesting result of the present paper is that even though we show the perturbation approach fails to predict the correct numerical coefficients for the asymptotic C dependence of the $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ in the continuum limit, the asymptotic dependence of $\Delta_{\rm PN}$ and $\omega_{\rm PN}$ on C as obtained within the zero-order perturbation approach [assumption (1) and even assumption (2)] is still functionally correct. Thus the perturbation approach might survive as a qualitative method of testing weak discrete systems. It remains an irrefutable fact that the perturbation approach led to a deep understanding of the nature of the $U_{\rm PN}$ in a discrete system.

ACKNOWLEDGMENT

This work is supported by part (S.F.) by the Deutsche Forschungsgemeinschaft (Fl 200/1-1).

---

* Electronic address: flach@buphy.bu.edu

[1] *Physics in One Dimension*, edited by J. Bernasconi and T. Schneider (Springer-Verlag, Berlin, 1981).
[2] *Dynamical Problems in Soliton Physics*. edited by S. Takeno (Springer-Verlag, Berlin, 1985).
[3] J. F. Currie, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, Phys. Rev. B **15**, 5567 (1977).
[4] N. Theodorakopoulos, W. Wünderlich, and R. Klein, Solid State Commun. **33**, 213 (1980).
[5] V. L. Pokrovsky, J. Phys. (Paris) **42**, 761 (1981).
[6] M. Peyrard and M. Remoissenet, Phys. Rev. B **26**, 2886 (1982).
[7] Y. Ishimori and T. Munakata, J. Phys. Soc. Jpn. **51**, 3367 (1982).
[8] J. A. Combs and S. Yip, Phys. Rev. B **28**, 6873 (1983).
[9] M. Remoissenet, Phys. Rev. B **33**, 2386 (1986).
[10] C. R. Willis, M. El-Batanouny, and P. Stancioff, Phys. Rev. B **33**, 1904 (1986).
[11] P. Stancioff, C. R. Willis, M. El-Batanouny, and S. Burdick, Phys. Rev. B **33**, 1912 (1986).
[12] S. E. Trullinger and K. Sasaki, Physica D **28**, 181 (1987).
[13] C. R. Willis and R. Boesch, Phys. Rev. B **41**, 4570 (1990).
[14] P. Woafo, T. C. Kofane, and A. S. Bokosah, J. Phys. Condens. Matter **4**, 3389 (1992).
[15] T. Munakata, Phys. Rev. A **45**, 1230 (1992).
[16] R. K. Dodd, J. C. Eilbeck, J. D. Gibbon, and H. C. Morris, *Solitons and Nonlinear Wave Equations* (Academic, London, 1982).
[17] S. E. Trullinger and R. M. DeLeonardis, Phys. Rev. A **20**, 2225 (1979).
[18] P. Tchofo Dinda, R. Boesch, E. Coquet, and C. R. Willis, Phys. Rev. B **46**, 3311 (1992).
[19] R. Boesch, P. Stancioff, and C. R. Willis, Phys. Rev. B **38**, 6713 (1988).
[20] R. Boesch and C. R. Willis, Phys. Rev. B **39**, 361 (1989).
[21] I. S. Gradshtein and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1965).
[22] M. Peyrard and H. Büttner, J. Phys. C. **20**, 1535 (1987).
[23] A. M. Dikande and T. C. Kofane, J. Phys. Condens. Matter **3**, 5203 (1991).
[24] P. Tchofo Dinda, R. Boesch, and C. R. Willis (unpublished).