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# Kink static properties in a discrete $\Phi^4$ chain with long-range interactions

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We study the discreteness effects on kink static properties in a one-dimensional anharmonic $\Phi^4$ chain with a long-range interaction potential of Kac-Baker type. Using the Dirac's second class constraints, we show that the discrete kink experiences the periodic Peierls-Nabarro (PN) potential whose barrier depends strongly on the range of interaction. Numerical calculations reveal that the dressing of the kink profile by the lattice effects lowers the PN potential and considerably increases its barrier. It is seen that the dressing and its effects tend to disappear when the range of interaction increases.

## I. INTRODUCTION

In recent years, considerable efforts have been concentrated on the propagation of nonlinear waves in a one-dimensional anharmonic lattice. Important new features have been outlined, which the more conventional continuum approach fails to describe adequately; for instance, the modulation of kink parameters obtained by Ishimori and Munakata in their perturbation scheme to describe the discrete sine-Gordon system,[1] the damped oscillatory motion and the lattice pinning effects of short topological solitons, the adiabatic dressing of kink, and the spontaneous emission of phonons.[2–13] In non-Hamiltonian and inhomogeneous lattices, the discreteness effects give rise to other interesting phenomena. Peyrard and Kruskal showed after numerical simulation that the velocity of a discrete kink driven by a low external force evolves by steps:[14] that is, for a large range of applied forces, the final velocity remains almost constant and then jumps to another value where it is again constant for a new range of the force. Those steps occur at some critical velocities for which the emission of phonons, due to lattice discreteness, is absent (e.g., the quasisteady states). It has also been shown that in presence of small external field and damping, a discrete kink moves like a damped-driven particle in the Peierls-Nabarro potential.[15,16] When the external field increases, it destroys the symmetry of the $\Phi^4$ substrate potential and a discrete asymmetric kink moves in a PN potential whose barrier is a decreasing function of the external field.[10] Recent studies reveal that a kink can be repelled by a point mass impurity in the discrete lattice,[17–19] a phenomenon which is absent in the continuum limit.

As consequences of these phenomena due to lattice discreteness, one observes a renormalization of kink diffusion constant and other thermodynamical properties of the lattice.[20–23,40] Interesting results have also been obtained in the dynamics of the two-component soliton in a discrete hydrogen-bonded chain.[24]

The efforts and results mentioned above have been limited to nearest-neighbor atomic interactions. In some materials, however, such as metals or ferroelectrics,[25,26] interatomic forces extend further than the nearest neighbors. In continuum medium interesting properties are observed in such systems.

Pnevmatikos showed that additional coupling between second-nearest neighbors causes subsonic solitonlike excitations[27] and mentioned the splitting and blowup of solitons due to competition between the first- and second-nearest-neighbor coupling.[28] A model of a nonlinear one-dimensional lattice with a long-range coupling of Lennard-Jones type was studied by Ishimori.[29] The results show that the force range parameter contributes to the dispersion relation. Moreover, the equations obtained from the model are classified into three types: the Benjamin-Ono equation, the Korteveg–de Vries equation and a third one whose analytic solution is unknown. Pokrovsky and Virosztek modified the Frenkel-Kontorova model by replacing the spatial second derivative in the sine-Gordon equation by an integral operator which contains both the short-range (local) and the long-range (nonlocal) interactions.[30] They came to the conclusion that the local theory cannot explain the observed finite exponent that appears in the density of solitons but, assuming a long-range (nonlocal) interaction, the theory can give a finite exponent at zero temperature. Another long-range potential is the well-known Kac-Baker potential,[31,32] in which the interaction between the particles falls off exponentially as the distance between them increases. It has been used by many authors to analyze the thermodynamics of systems such as the Ising,[31,32] the Pott,[33] and the $\Phi^4$ (Ref. 34) models. It has also been used to investigate the effect of the range of interaction on the properties of solitonlike excitations in a one-dimensional anharmonic nonmagnetic chain[35] and magnetic Heisenberg chain.[36] One should refer to Ref. 26 for another presentation and analysis of long-range character of interaction between particles.

Because of the amount of interesting phenomena appearing in the continuum long-range interaction systems, it is convenient to investigate the discreteness effects in such systems. In a recent paper,[37] following earlier work by Willis, El-Batanouny, and Stancioff on the discrete sine-Gordon chain,[9] we have used a discrete $\Phi^4$ chain with long-range interaction of Kac-Baker type to present the first results on the subject. An important conclusion obtained was that the barrier of the Peierls-Nabarro (PN) potential vanishes as the range of interaction increases.

In this paper, we complete the previous study by analyzing the dressing in terms of the interaction parameter. We discuss the dressing effects on the static properties of the kink in the discrete lattice. The plan of the paper is as follows.

Section II deals with the presentation of the long-range interaction chain and the resulting kink solution. The details related to the mathematical formalism and the results of the preceding paper are given in Sec. III. A matrix equation for the discrete fluctuations (or dressings) correcting the kink profile is established. A numerical analysis is used to evaluate the spatial variation of dressing and to compute its effects on the PN potential. We present our conclusions in Sec. IV.

## II. THE $\Phi^4$ CHAIN WITH LONG-RANGE INTERACTION AND ITS KINK SOLUTION

The discrete model under consideration consists of a one-dimensional chain of $N$ ions, each of mass $m$, with an equilibrium spacing $b$ between neighboring ions. $m$ and $b$ are set equal to unity. The ions are assumed to interact through a long-range interatomic potential of the Kac-Baker type. Thus, the interaction force between the particles of the chain falls off exponentially with the separation. The long-range coupling coefficient has the form

$$V_{ij}=\frac{J(1-r)r^{|i-j|}}{2r} , \tag{2.1}$$

where $J$ is the elastic constant of the lattice and $r$ defines the range of interaction, with $0 \le r < 1$. $|i-j|$ is the distance between the ions of sites $i$ and $j$. The virtue of this particular interaction, commonly encountered in physical systems such as the Ising or ferromagnet lattices, is that the range of interaction can be varied continuously. In addition, each particle lies in the $\Phi^4$ substrate potential so that the total potential energy of the discrete chain is

$$U=\frac{1}{2}\sum_{j\neq i} V_{ij}(y_i-y_j)^2+\frac{1}{4}\sum_i (y_i^2-1)^2 \tag{2.2a}$$

and the Hamiltonian is given by

$$H=\frac{1}{2}\sum_i \dot{y}_i^2+U , \tag{2.2b}$$

where the summation is over the $N$ particles. $y_i$ is the displacement field of the $i$th ion from its equilibrium site $x_i=i$.

The prefactor $(1-r)$ in Eq. (2.1) is chosen to ensure that the total potential experienced by one atom due to all others is finite in the thermodynamic limit (when $N$ goes to infinitive). This is equal to $J$. The range of interaction increases with $r$. For $r=0$, the model reduces to a nearest-neighbor problem. The limit $r \to 1$, which should be taken only in the thermodynamic limit, corresponds to the infinite-range problem.

The equation of motion derived from Eq. (2.2) is

$$\ddot{y}_i-(1-2J)y_i+y_i^3=L_i , \tag{2.3}$$

where the auxilliary quantity $L_i$, a function of the set of displacements of all ions (other than the $i$th ion), is defined as

$$L_i=\frac{J(l-r)}{r}\sum_{j\neq i} r^{|i-j|}y_j . \tag{2.4}$$

Following the recursive relation

$$(r+r^{-1})L_i=L_{i+1}+L_{i-1} + \frac{J(1-r)}{r}(y_{i+1}+y_{i-1}-2ry_i) , \tag{2.5}$$

we make the continuum approximation $y_i(t) \to y(x,t)$ and $L_i(t) \to L(x,t)$, to obtain the partial differential equation

$$ry_{xxtt}+[J(1+r)-r]y_{xx}+r(y^3)_{xx} -(1-r)^2(y_{tt}+y^3-y)=0 . \tag{2.6}$$

Equations (2.3) and (2.6) have two phonon solutions: oscillations about the top ($y=0$) of the double well and the oscillations about the bottom ($y=\pm 1$) of the well.[34,40] For $r=0$, Eq. (2.6) reduces to the well-known $\Phi^4$ continuum equation.[39]

Neglecting the fourth-order term in limit of the continuum approximation, Eq. (2.6) leads to large amplitude kink solutions $y(x,t)$ given by the implicit formula[34]

$$\pm\frac{x-Vt}{\sqrt{2}\xi} =-3\left[\frac{\sigma}{2}\right]^{1/2}\sinh^{-1}\left[\frac{2\sigma}{1+\sigma}\right]^{1/2}y +(1+3\sigma)^{1/2}\tanh^{-1}\left[\left[\frac{1+3\sigma}{1+\sigma+2\sigma y^2}\right]^{1/2}y\right] , \tag{2.7}$$

where

$$\xi^2=\frac{J(1+r)-r-V^2(1-r)^2}{(1-r)^2} \tag{2.8a}$$

and

$$\sigma=\frac{r}{(1-r)^2\xi^2} . \tag{2.8b}$$

$y(x,t)$ is a topological soliton solution with the width measured by $\xi$ and that propagates with the constant velocity $V$ in absence of thermal effects or perturbations. The positive (negative) sign corresponds to kink (antikink).

In Ref. 37, we have simplified the implicit kink solution (2.7) by the following hyperbolic tangent wave form

$$y_K(x,t)=\tanh[K(x-Vt)] , \tag{2.9}$$

where

$$K^2=\frac{1}{2C^2(r)} , \tag{2.10a}$$

with

$$C^2(r)=\frac{J(1+r)-r}{(1-r)^2} . \tag{2.10b}$$

$C(r)$ is the speed of sound and $L_a = K^{-1} = \sqrt{2}\xi$ $[V \ll C(r)]$ defines the spatial extension of kink in the nonrelativistic regime. It increases indefinitely as the range of interaction increases (see Fig. 1). Since we are dealing with a discrete kink (short kink), our calculations are limited to small values of the range parameter $r$.

There are two facts which support the validity of the approximation (2.9). First, the soliton profile given by Eq. (2.7) suffers slightly because of the approximation. The slight difference between the two profiles decreases as $r$ decreases and for long-range interaction with small amplitude (the more discrete kink), the profiles are quite identical. Second, the soliton energy obtained in the continuum limit from Eq. (2.9) is

$$E_K = \frac{2\sqrt{2}}{3}\xi + \frac{2\sqrt{2}V^2}{3\xi} , \tag{2.11a}$$

which approximately corresponds to

$$E_K = \frac{2\sqrt{2}}{3}\xi\left[1 + \frac{189}{640}\sigma - \frac{831}{8960}\sigma^2\right] + \frac{\sqrt{2}V^2}{\xi}\left[\frac{2}{3} + \frac{\sigma}{15} - \frac{17}{252}\sigma^2\right] , \tag{2.11b}$$

derived from the implicit solution (2.7) (see Ref. 34). However, one can note that the error between the two expressions increases with an increasing range of interaction. For instance, for $r = 0.1$, the error is 2.9%; for $r = 0.4$, it is only 5.5% which is still acceptable. But, for $r = 0.5$, the error reaches 12.6% which already corresponds to a poor approximation. Fig. 2 shows the plots, for comparison, of expressions (2.11a) and (2.11b) as functions of the long-range interaction parameter.

## III. ANALYSIS OF DRESSINGS AND THE EFFECTS ON THE PN POTENTIAL IN A $\Phi^4$ CHAIN WITH LONG-RANGE INTERACTION

In line with the discrete kink formalism,[9] the displacement field $y_i$ is separated into a single kink $y_K^i[X(t)]$ plus the dressing term $\psi_i(t)$ which accounts for the discrete correction of the continuum kink and for phonons radiated by the kink while propagating in the lattice. That is, we set

$$y_i = y_K^i[X(t)] + \psi_i(t) , \tag{3.1}$$

where

$$y_K^i[X(t)] = \tanh\{K[i - X(t)]\}$$

denotes the continuum kink at the discrete lattice point $i$. The dynamical variable $X(t)$ represents the kink center position. We remind the reader that in the continuum limit, $X(t)$ is linearly time dependent [i.e., $X(t) = Vt$]. As it has been shown earlier [see Ref. 37 and Eq. (3.4) hereafter], this is not the case in the discrete limit where $X(t)$ possesses a rich dynamical behavior.[11,14,20]

Decomposition (3.1) adds two more degrees of freedom to the system, corresponding to the collective coordinate $X(t)$ and its conjugate momentum $P$. Then, in order to conserve the original number of degrees of freedom, the system is subjected to two constraints, which give a functional link between the new variables and the field $y_K^i$. They are

$$C_1 = \sum_i y_K^{i(1)}\psi_i = 0$$

and (3.2)

$$C_2 = \sum_i y_K^{i(1)} p_i = 0 .$$

The subscript (1) stands for the derivative with respect to $X$. $p_i$ is the conjugate momentum of $\psi_i$.

Constraints $C_1$ and $C_2$ tend to minimize the fluctuations in the vicinity of the kink's center and allow a canonical transformation of the original coordinates $y_i$ and $\dot{y}_i$ to new variables $X$, $P$, $\psi_i$, and $p_i$. They have been shown to be second-class constraints in Dirac's terminology[38,41,42] since their Poisson brackets do not yield zero, thus violating the requirement that $C_1 = 0$ and $C_2 = 0$. Because of these constraints, the formalism developed by Dirac's for constrained dynamical systems has to be ap-

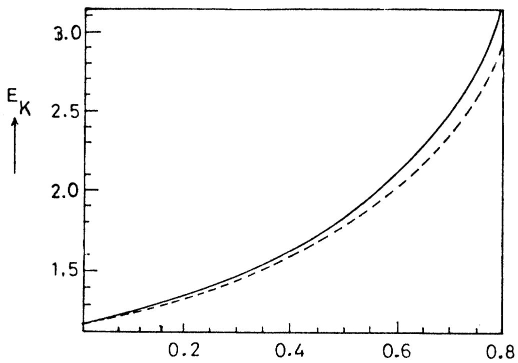


FIG. 2. Comparison, with respect to $r$, between the soliton energy obtained from the implicit solution (full curve) to that obtained from the approximated wave form (dashed curve) for $J = 1.5$.

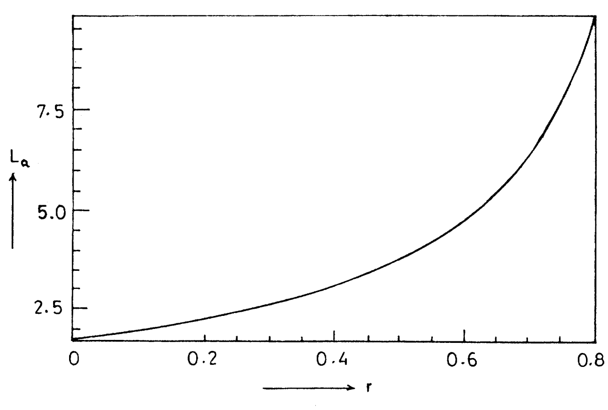


FIG. 1. Kink width $L_a$ as function of the long-range interaction parameter for $J = 1.5$.

plied in order to derive the evolution equations of the variables $X$, $P$, $\psi_i$, and $p_i$.[37]

In Ref. 37, we have used this formalism to show that the kink of the discrete $\Phi^4$ chain with long-range interaction is subjected to the potential force

$$\partial U/\partial X=\sum_i y_K^{i(1)}[(\psi_i+y_K^i)^3-(1-2J)(\psi_i+y_K^i)-L_i)] , \tag{3.3}$$

where $L_i$ is now associated to $\psi_j+y_K^j$. Neglecting the $\psi_i$ contribution, we show that $U(X)$ can be reduced to the Fourier series

$$U(X)=U_0+\sum\frac{E_n}{2\pi n}\cos(2\pi nX)\approx U_0+\frac{E_1}{2\pi}\cos(2\pi X) \tag{3.4}$$

with

$$E_n=-\frac{r}{6(1-r)^2}\left[\frac{J(1+r)-r}{r}I_n+J_n\right] ,$$

where

$$I_n=8n^2\pi^3K^2\sinh^{-1}(n\pi^2/K)[2(q_n+1)/3-4(q_n+1)(q_n+4)/15] ,$$

$$J_n=24K^4\pi\sinh^{-1}(n\pi^2/K)[-54(q_n+1)(q_n+4)(q_n+9)(q_n+16)/567+788(q_n+1)(q_n+4)(q_n+9)/315 -142(q_n+1)(q_n+4)/15+8(q_n+1)/3] ,$$

and

$$q_n=(\pi n/K)^2 .$$

The quantity $E_{\rm PN}=E_1/\pi$ is the PN pinning potential barrier, well known in the theory of crystal dislocations.[43] It vanishes as the elastic constant $J$ and the range of interaction increase (see Fig. 1 of Ref. 37 and Fig. 5 hereafter). When the kink width increases, $E_1$ vanishes and the kink potential energy reduces to the $X$-independent term $U_0$. The effect of the lattice discreteness is characterized by a shift in the kink rest energy. In the first approximation, this shift is obtained after a fourth-order Taylor expansion of the auxilliary quantity $L_i$ while deriving the kink potential energy (see Ref. 40). $U_0$ is then given by the expression

$$U_0=E_K^{(0)}-\frac{2rK^3}{15(1-r)^2}\left[\frac{J(1+r)-r}{3r}-\frac{1}{7}\right] , \tag{3.5}$$

where $E_K^{(0)}$ is the kink rest energy in the continuum limit. It therefore appears that the kink rest energy in the discrete lattice is less than the continuum value. Such lowering has also been obtained recently by other authors.[22,23] It should certainly be more pronounced if one takes into account the dressing contribution while calculating the kink rest energy (see, for instance, Fig. 4 where the dressing lowers the level of the PN potential).

In the dynamical regime, the velocity of the kink is therefore modulated by the PN potential. At small velocities, the kink may be pinned in the PN well. When this happens, the kink oscillates about the bottom of the potential with the frequency $\omega_p$ defined as follows:

$$\omega_P=(2\pi E_1/M_0)^{1/2} , \tag{3.6}$$

where $M_0=4K/3$ is the kink dimensionless mass (see Ref. 37). $\omega_P$ is also a decreasing function of the long-range interaction parameter $r$.

In view of analyzing the dressing amplitude (ignoring the phonons part) and its effects on the PN potential seen by a kink, one has to solve the problem obtained after extremization of the potential (2.2a) with respect to the dressing field $\psi_i$ [after substitution of $y_i$ by $y_K^i(X)+\psi_i$]. For a kink centered at the equilibrium position of the periodic PN potential, one obtains after some algebra the matrix problem

$$A\psi=F , \tag{3.7a}$$

where $\psi$ and $F$ are column matrices respectively defined by

$$\psi=\begin{bmatrix}\cdot\\ \cdot\\ \psi_i\\ \cdot\\ \cdot\end{bmatrix} , \tag{3.7b}$$

$$F=\begin{bmatrix}\cdot\\ \cdot\\ F_i\\ \cdot\\ \cdot\end{bmatrix} , \tag{3.7c}$$

with

$$F_i=r[(y_k^{i+1})^3+(y_K^{i-1})^3]+[J(1+r)-r](y_K^{i+1}+y_K^{i-1}) -(r^2+1)(y_K^i)^3+[r^2+1-2J(1+r)]y_K^i . \tag{3.7d}$$

$A$ is a tridiagonal matrix with elements defined by

$$(A)_{il}=-[3r(y_K^{i+1})^2-r+J(1+r)]\delta_{i,l-1} +[3(r^2+1)(y_K^i)^2+2J(1+r)-(r^2+1)]\delta_{i,l} -[3r(y_K^{i-1})^2-r+J(1+r)]\delta_{i-1,l} , \tag{3.8}$$

where $\delta_{i,l}$ is the Kronecker delta.

In this state, the constraint $C_1$ is automatically satisfied in the calculation of $\psi_i$ from eq. (3.7). This follows the parity of matrix elements and $F_i$. But, for a kink in nonequilibrium points of the lattice, a Lagrange multiplier $\alpha(X)$ which multiplies the constraint is required. Indeed, in nonequilibrium points, the PN force draws the kink and prevents a static dressing. This is done by adding the constraint $C_1$ with an undetermined multiplier to the original potential.[10] That is,

$$U \to U + \alpha(X) \sum y_K^{i(1)} \psi_i \ . \tag{3.9}$$

This procedure, known as quasistatic approach, provides the external force to balance the PN force in order to keep the dressing static. The minimization of the new potential leads to

$$A\Psi = F - \alpha(X)(r^2+1) Y_K^{(1)} \ , \tag{3.10}$$

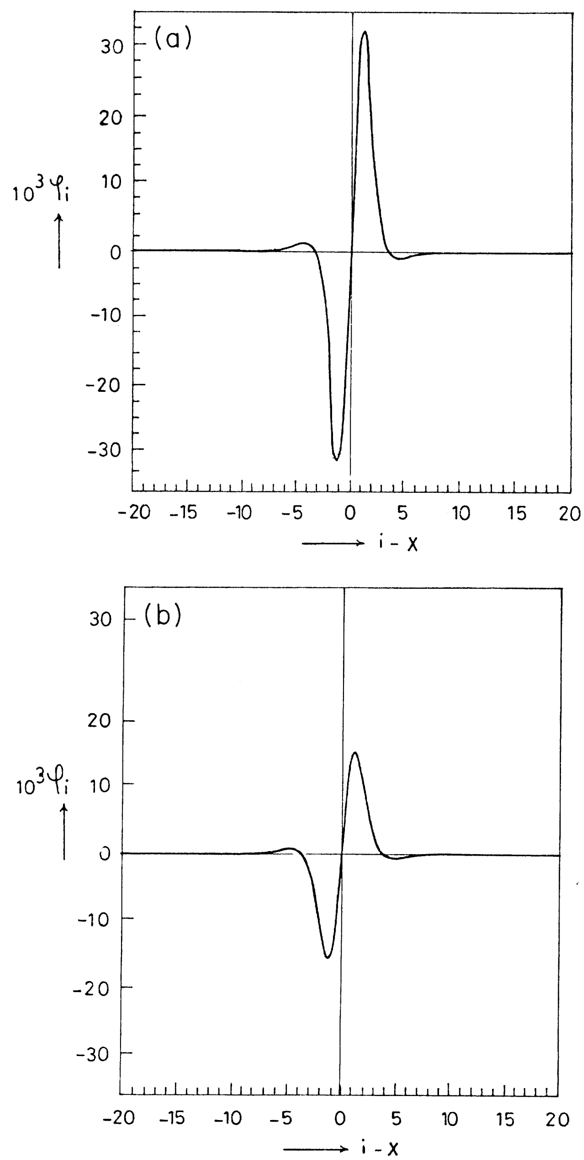


FIG. 3. Dressing $\psi_i$ ($\times 10^3$) as a function of the distance from the kink center for elastic constant $J=1.5$ and (a) $r=0$ and (b) $r=0.1$.

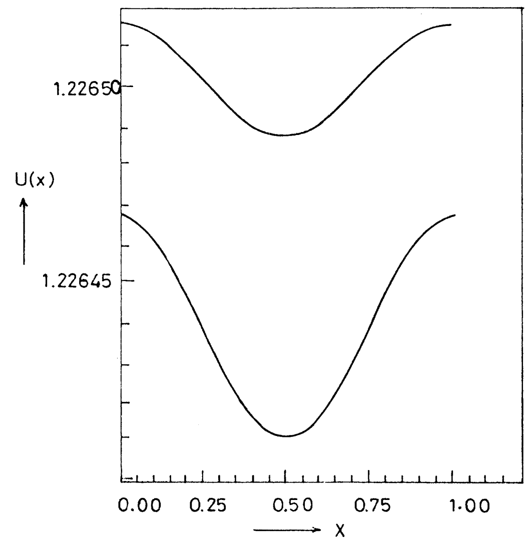


FIG. 4. Peierls-Nabarro potential $U(X)$ vs the position $X$ in a unit cell of the lattice for $r=0.05$ and $J=1.5$. The upper curve is the potential without dressing contribution and the lower one includes the dressing effects. Due to dressing, the potential is lowered and its height is increased (see Fig. 5).

where

$$Y_K^{(1)} = \begin{bmatrix} \vdots \\ y_K^{i(1)} \\ \cdot \\ \cdot \end{bmatrix} .$$

Solving Eq. (3.10) for $\Psi$ and multiplying the obtained equation by the transposed $[Y_K^{(1)}]^T$ of the column matrix $Y_K^{(1)}$, we use the constraint $C_1$ to obtain

$$\alpha(X) = \frac{1}{r^2+1} [Y_K^{(1)}]^{\mathrm{T}} A^{-1} F ([Y_K^{(1)}]^{\mathrm{T}} A^{-1} Y_K^{(1)}) \ . \tag{3.11}$$

The static dressing is then obtained by substituting Eq. (3.11) into Eq. (3.10).

For the numerical calculation, we have considered a chain of $N=200$ particles. The kink is located at the

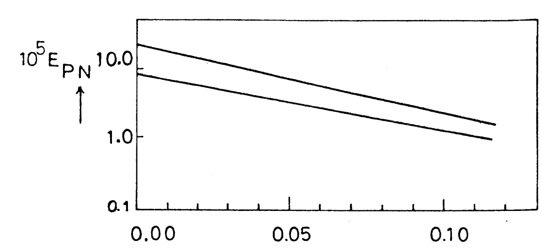


FIG. 5. Log plot of the PN barrier $E_1$ ($\times 10^5$) as a function of the long-range interaction parameter $r$. The upper curve for the barrier with dressing and the lower for the barrier without the inclusion of dressing (for $J=1.5$).

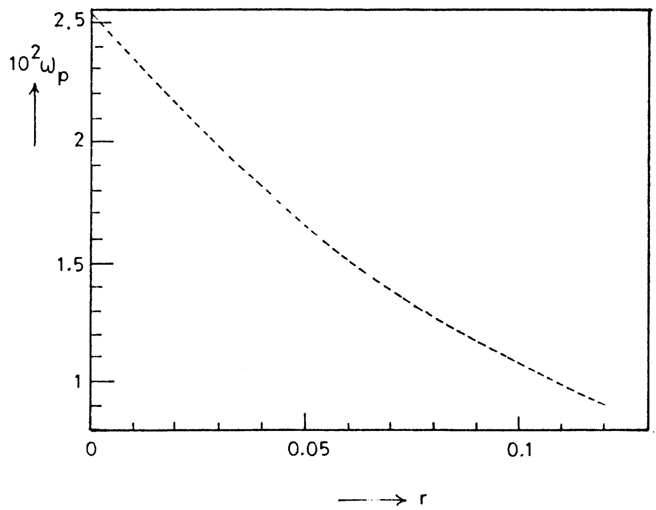


FIG. 6. The pinning frequency $\omega_P$ (in hundreds) as a function of $r$ for $J = 1.5$.

middle of the chain in order to avoid the end effects. Since the dressings are localized around the kink core, we have truncated the matrix $A$ by attributing the value zero to $\psi_i$ when $i$ is not contained in the integer domain

$$[\mathrm{int}(5L_a), N - \mathrm{int}(5L_a)] ,$$

where $\mathrm{int}(5L_a)$ is the integer obtained from the conversion of real $5L_a$ to the integer type. The parameter $L_a$ being the kink spatial extension.

Figure 3 shows the plot of dressing versus the distance $i - X$ from the center of kink. It follows that the constraint $C_2$ is satisfied since the product $y_K^{i(1)}\psi_i$ is an odd function. We also see that the amplitude of the dressing decreases when the range of interaction increases [compare Figs. 3(a) and 3(b)].

When $\psi_i$ is added to $y_K^i$, one obtains around the kink center a small deviation from the zeroth-order kink profile. Although the deviation is small, even for a kink width equal to the lattice spacing, it has considerable effect on the PN potential. Indeed, the inclusion of dressing lowers the level of the PN potential and considerably increases its amplitude. This is seen in Fig. 4 where we have calculated for 200 lattice particles the potential $U$ [see Eq. (2.2a)] using first the kink solution $y_K^i(X)$ (the upper curve) and second the dressed profile $y_K^i(X) + \psi_i$ (the lower curve). The lowering, which has been shown analytically for the kink rest energy near the continuum limit, is due to the discrete nature of the lattice.

The PN barrier $E_1$ and the PN frequency $\omega_P$ have been calculated for various values of the range of interaction. The results are shown in Figs. 5 and 6. In Fig. 5, we have given a log plot of the PN barrier (with and without dressing) as a function of the long-range interaction parameter $r$. Both Figs. 5 and 6 show the decreasing behavior of $E_1$ and $\omega_P$ when $r$ increases. This result confirms that presented in Fig. 1 of Ref. 37 from the analytic expression (3.4).

## IV. CONCLUSION

In this paper, we have studied the strongly anharmonic $\Psi^4$ lattice complicated by the addition of the long-range interatomic coupling in the case where the discreteness effects cannot be neglected. The virtue of the specific interaction potential chosen, the Kac-Baker type, is that the range of interaction can be varied continuously.

We have shown that the lattice generalized potential depends strongly on the long-range interaction parameter $r$. As the range of interaction increases, the pinning and trapping processes tend to disappear since the PN barrier decreases rapidly. We have also shown that the dressing lowers the PN potential and increases the PN barrier. The dressing amplitude tends to disappear when the range of interaction increases.

The studies similar to those considered here have been carried out for the sine-Gordon model with the Kac-Baker long-range interaction potential. The closed-form (implicitly) kink solutions have already been obtained.[44] Extensions should also concern other laws of long-range interparticle interactions such as the power laws (i.e., the Coulomb repulsion or the dipole-dipole interaction of charges particles) where interesting results have already been obtained for the Frenkel-Kontorova model.[26]


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