Sine-Gordon kinks on a discrete lattice. I. Hamiltonian formalism

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We derive a complete Hamiltonian formalism for a kink on a one-dimensional discrete lattice in which the position of the center of the kink appears as one of the canonical variables. Our method is a generalization to the discrete lattice of the method used in field theory to introduce the soliton as a canonical degree of freedom. The derivation is valid for a particle chain in a periodic potential when there exists a solitary-wave solution in the continuum limit. We show that the discrete lattice is responsible for an adiabatic dressing of the kink and for spontaneous emission of phonons. In the limit where the effective length of the kink is much larger than the interparticle spacing the kink experiences the well-known periodic Peierls-Nabarro potential. In the case of a short kink, the discrete lattice causes the continuum kink configuration to be adiabatically dressed, leading to a renormalization of the Peierls-Nabarro potential and in turn to an enhancement of corresponding small-amplitude oscillatory frequency. In addition, we formally derive an equation that describes the radiation of phonons by the moving kink, an effect of the lattice discreteness.

I. INTRODUCTION

The striking connection between the properties of solitary waves and many nonlinear phenomena in physics has led to a host of related publications[1] in the past decade. These investigations have provided valuable information as to the applicability and limitations of this class of nonlinear entities. Recently it has been demonstrated that systems involving a minimum distance scale, such as an underlying lattice, give rise to interesting phenomena in the structural and dynamic properties of solitary waves or kinks absent in their continuum counterparts.[1–10] As a matter of fact, investigations of these properties have become fashionable and challenging. Aubry was the first to recognize the manifestations of discreteness in the static properties of solitons, or kinks.[2] Through an elegant mathematical approach he was able to demonstrate the existence of a pinned regime in discrete kinks, as well as a depinning transition that can occur in incommensurate systems at some critical value of the coupling coefficient. Furthermore, Currie *et al.*[3] have demonstrated the possibility of radiative damping for moving kinks that would otherwise exhibit uniform motion under continuum conditions. These initial studies prompted investigations along two directions: pinning and radiation, as well as their interrelationship. Since the kink-radiation interaction, which leads to spontaneous emission, is an intrinsically discrete effect, attempts to bypass discreteness in some way and to resort to a continuum formulation have failed either to predict such manifestations or to provide a coherent picture of the kink's diffusive motion in the presence of radiation. In a recent publication Combs, and Yip (CY),[4] recognizing these shortcomings, made significant progress toward achieving a fundamental formulation of the problem of a kink on a discrete lattice by using some of the techniques employed in field theory to introduce a soliton as a distinct degree of freedom.

In this paper we develop for the first time a complete Hamiltonian dynamics for $2N+2$ canonical variables; two of the variables are the kink coordinate and associated momentum, while the remaining $2N$ variables describe the radiation field, as well as the deviations from the continuum soliton solutions. Since the Frenkel-Kontorova model,[11] which is the discrete analogue of the sine-Gordon system, consists of N particles, the introduction of two new canonical variables requires invoking two constraints. Our formalism is an extension of field-theoretical techniques to the discrete kink problem. In essence, we apply the approach developed by Tomboulis,[12] to introduce a soliton degree of freedom as a canonical variable in field theory to the problem of a kink on a discrete lattice. The method we develop is applicable to any problem where a single-particle periodical potential has a soliton solution in the continuum limit. In this paper we develop the theory for the sine-Gordon potential. We follow a nonrelativistic formulation of the kink motion since, on the one hand, most of the relevant physical applications belong to that regime, and on the other hand, the formal requirements of a relativistic kink Hamiltonian dynamics tend to obscure some of the discrete lattice effects.

The organization of this paper will be as follows. In Sec. II we introduce the necessary constraints and derive the canonical transformation to a Hamiltonian that includes the kink as two of the $2N+2$ canonical variables. We derive the equations of motion in Sec. III. In Sec. IV we discuss some significant special cases. We compare our approach with previous work, especially with that of Combs and Yip, in Sec. V. Section VI contains the summary and conclusions. In the Appendix we explicitly evaluate the integrals that appear in the Fourier expansion of the "bare" Peierls-Nabarro potential.[13]

II. DISCRETE CANONICAL TRANSFORMATION AND HAMILTONIAN

The Lagrangian for the sine-Gordon equation is

$$L=\frac{m}{2}\sum_{n=1}^{N}\dot{x}_n^2-\tfrac{1}{2}\mu\sum_{n=1}^{N}(x_{n+1}-x_n)^2-\frac{W}{2}\sum_{n=1}^{N}\left[1-\cos\left[2\frac{\pi x_n}{a}\right]\right], \quad (2.1)$$

where an overhead dot indicates differentiation with respect to time, a is the period of the periodic potential, $W/2$ the amplitude of the periodic potential, μ is the force constant of the springs, m is the mass of the particles, and x_n is the displacement of the nth particle from the nth trough of the substrate potential. When dimensionless variables are introduced in Eq. (2.1) the Lagrangian becomes

$$L\equiv(a^2\mu)^{-1}L=\tfrac{1}{2}\sum_{l=1}^{N}\dot{Q}_l^2-\tfrac{1}{2}\sum_{l=1}^{N}(Q_{l+1}-Q_l)^2-\frac{1}{4l_0^2}\sum_{l=1}^{N}[1-\cos(2\pi Q_l)], \quad (2.2)$$

where $Q_l\equiv x_l/a$, the dimensionless time is $\tau\equiv\frac{1}{2}\omega_m t$, the square of the frequency ω_m is $\omega_m^2\equiv4\mu/m$, the square of the dimensionless coupling constant l_0 is $l_0^2=(\pi/2)^2(\omega_m^2/\omega_s^2)$, and the square of the frequency ω_s is $\omega_s^2=2\pi^2a^{-2}(W/m)$. A large value of l_0 corresponds to the case where the harmonic forces between the particles are larger than the force due to the periodic potential of the substrate.

We now define new variables q_l and their time derivatives $\dot{q}_l$:

$$Q_l\equiv q_l+f_l(X),$$

$$\dot{Q}_l=\dot{q}_l+\dot{X}f_l^{(1)}(X),$$

where

$$f_l=(2/\pi)\tan^{-1}(e^{\pi(l-X)/l_0}) \quad (2.3)$$

is the single-soliton solution of the continuum sine-Gordon equation. We will use the notation $f_l^{(i)}$ to indicate $d^if_l(X)/dX$, where X is the position coordinate for the soliton. We now have $N+1$ coordinates: the N q_l's and the soliton variable X. We seek a Hamiltonian description with these coordinates and their canonically conjugate momenta. The original problem had $2N$-independent variables, but we now have $2N+2$ variables. Therefore, we must introduce two constraints in order to achieve a canonical transformation of the original theory. Tomboulis has shown that the introduction of a soliton in field theory can be cast as a canonical transformation by using Dirac brackets. The application of this method to a discrete lattice involves essentially a change of the continuous field variables of Ref. 12 to discrete lattice variables. The required constraints on the discrete variables are

$$C_1=\sum_{l=1}^{N}f_l^{(1)}q_l=0,\quad C_2=\sum_{l=1}^{N}f_l^{(1)}p_l=0, \quad (2.4)$$

where p_l is the momentum conjugate to q_l, i.e., $p_l=\partial L/\partial\dot{q}_l=\dot{q}_l$. We can motivate the introduction of the constraints in part by the following argument. Let us suppose that we would like the kinetic energy of our new Hamiltonian to consist of a sum of $N+1$ terms, one of which is the soliton kinetic energy, and the remaining N terms are a sum of N kinetic energies, one for each particle, with no cross terms between the soliton kinetic energy and the particle kinetic energies. The total kinetic energy in terms of the variables defined by Eq. (2.3) is then

$$\tfrac{1}{2}\sum_{l=1}^{N}\dot{Q}_l^2=\tfrac{1}{2}\sum_{l=1}^{N}[\dot{q}_l^2+2\dot{q}_l\dot{X}f_l^{(1)}+\dot{X}^2(f_l^{(1)})^2]. \quad (2.5)$$

If we require that $\sum_l\dot{q}_lf_l^{(1)}=0$, then Eq. (2.5) becomes

$$\tfrac{1}{2}\sum_{l=1}^{N}\dot{Q}_l^2=\tfrac{1}{2}\sum_{l=1}^{N}\dot{q}_l^2+\tfrac{1}{2}M\dot{X}^2, \quad (2.6)$$

where $M\equiv\sum_l(f_l^{(1)})^2$ plays the role of the dimensionless mass of the soliton. Note that our requirement $\sum_l\dot{q}_lf_l^{(1)}=0$ is just the constraint C_2. From the definition of the conjugate momentum we have

$$P_l=p_l+P,$$

where

$$P_l=\frac{\partial L}{\partial\dot{Q}_l}=\dot{Q}_l,\quad p_l=\frac{\partial L}{\partial\dot{q}_l},\quad P=\frac{\partial L}{\partial\dot{X}}=M\dot{X}, \quad (2.7)$$

and the kinetic energy in terms of the momenta is

$$\tfrac{1}{2}\sum_{l=1}^{N}\dot{Q}_l^2=\tfrac{1}{2}\sum_{l=1}^{N}p_l^2+\frac{P^2}{2M}. \quad (2.8)$$

Next we show that the transformation from the $2N$ Q_l's and P_l's to the $2N$ q_l's and p_l's plus P and X is a canonical transformation when the two constraints $C_1=0$ and $C_2=0$ are invoked. The old variables satisfy the canonical Poisson bracket relations

$$\{Q_l,Q_n\}=\{P_l,P_n\}=0,\quad\{Q_l,P_n\}=\delta_{ln}. \quad (2.9)$$

Consider the new set of variables q_l, p_l, X, and P and assume for the moment that q_l and p_l satisfy

$$\{q_l,p_n\}=\delta_{ln}.$$

However, as a consequence the Poisson bracket of the constraints satisfy $\{C_1,C_2\}=\sum_{l=1}^{N}(f_l^{(1)})^2=M(X)$ which violates our requirement that $C_1=0$ and $C_2=0$. In Dirac's terminology[14] these are second-class constraints. To make the constraints strong requires a modification of the conventional brackets. The Hamiltonian formalism for a constrained system leads to a new canonical bracket

$$\{q_i,p_j\}=\delta_{ij}-\{q_i,C_\alpha\}(\{C_\alpha,C_\beta\})^{-1}\{C_\beta,p_j\}=\delta_{ij}-M^{-1}f_i^{(1)}(X)f_j^{(1)}(X), \quad (2.10)$$

where α and β take the values 1 and 2. We also set $\{X,P\}=1$, while all other Poisson brackets vanish.

Next we substitute $Q_l=q_l+f_l(X)$ and $P_l=p_l+P$ in the Poisson bracket relations of Eq. (2.9). When we use Eq. (2.10), $\{X,P\}=1$, and the constraints given by Eq. (2.4) to evaluate the Poisson brackets of Eq. (2.9), we find that the relations of Eq. (2.9) are satisfied. Consequently, the transformation to the new variables q_l, p_l, X, and P is canonical and the new dimensionless Hamiltonian is

$$H=\frac{P^2}{2M}+\frac{1}{2}\sum_{l=1}^{N}p_l^2+\sum_{l=1}^{N}V(q_l+f_l)\ , \tag{2.11a}$$

where

$$V(q_l+f_l)=\frac{1}{2}(q_{l+1}+f_{l+1}-q_l-f_l)^2+\frac{1}{4l_0^2}\{1-\cos[2\pi(f_l+q_l)]\}\ , \tag{2.11b}$$

with the canonical brackets in Eq. (2.10) and $\{X,P\}=1$. As a consequence of the modification of the brackets in Eq. (2.10) we find that $\{C_1,C_2\}=0$, as it must if the constraints $C_1=0$ and $C_2=0$ are to be satisfied.

III. EQUATIONS OF MOTION

We obtain the equations of motion for our $2N+2$ canonical variables from the Poisson bracket relation

$$\dot{O}=\{O,H\}\ , \tag{3.1}$$

where O is a function of the $2N+2$ canonical variables and does not depend explicitly on time. We use the relationship which follows from Eq. (2.10),

$$\{p_l,g(q)\}=-\frac{\partial g}{\partial q_l}+\frac{f_l^{(1)}(X)}{M}\sum_{l=1}^{N}f_{l'}^{(1)}(X)\frac{\partial g}{\partial q_{l'}}\ , \tag{3.2a}$$

$$\{q_l,g(p)\}=-\frac{\partial g}{\partial p_l}+\frac{f_l^{(1)}(X)}{M}\sum_{l'=1}^{N}f_{l'}^{(1)}(X)\frac{\partial g}{\partial p_{l'}}\ . \tag{3.2b}$$

The equations of motion for q_l and X are

$$\dot{q}_l=\{q_l,H\}=p_l-\frac{f_l^{(1)}(X)}{M}\sum_{l'=1}^{N}f_{l'}^{(1)}(X)p_{l'}=p_l\ , \tag{3.3a}$$

$$\dot{X}=\{X,H\}=\frac{P}{M}\ , \tag{3.3b}$$

where the second equality in Eq. (3.3a) follows from $C_2=0$. The equations of motion for p_l and P are then

$$\dot{p}_l=\ddot{q}_l=\{p_l,H\}=q_{l+1}+f_{l+1}+q_{l-1}+f_{l-1}-2(f_l+q_l)-\frac{\pi}{2l_0^2}\sin[2\pi(f_l+q_l)]-\frac{1}{M}f_l^{(1)}\sum_{l'=1}^{N}f_{l'}^{(1)}\left[q_{l'+1}+f_{l'+1}+q_{l'-1}+f_{l'-1}-2(f_{l'}+q_{l'})-\frac{\pi}{2l_0^2}\sin[2\pi(f_{l'}+q_{l'})]\right]\ , \tag{3.4a}$$

$$\dot{P}=\{P,H\}=\frac{P^2}{2M^2}\frac{dM}{dX}+\sum_{l=1}^{N}f_l^{(1)}\left[q_{l+1}+f_{l+1}+q_{l-1}+f_{l-1}-2(q_l+f_l)-\frac{\pi}{2l_0^2}\sin[2\pi(f_l+q_l)]\right]\ , \tag{3.4b}$$

where we use Eq. (3.2b) to obtain (3.4a). We obtain the equation for $\ddot{X}$ by substituting

$$\dot{P}=M\ddot{X}+\dot{M}\dot{X}=M\ddot{X}+\dot{X}^2\frac{dM}{dX} \tag{3.5}$$

into Eq. (3.4b) which becomes

$$\ddot{X}+\frac{1}{2}\dot{X}^2\frac{d\ln M}{dX}=(1/M)\sum_{l=1}^{N}f_l^{(1)}\left[q_{l+1}+f_{l+1}+q_{l-1}+f_{l-1}-2(q_l+f_l)-\frac{\pi}{2l_0^2}\sin[2\pi(q_l+f_l)]\right]. \tag{3.6}$$

Equation (3.6) is the equation of motion for the soliton degree of freedom in terms of the q_l's. The right-hand side of Eq. (3.6) constitutes a "generalized potential" which depends on X through the $f_l(X)$ and also depends on the q_l's. When we substitute the right-hand side of Eq. (3.6) in Eq. (3.4a), we obtain

$$\ddot{q}_l=q_{l+1}+f_{l+1}+q_{l-1}+f_{l-1}-2(f_l+q_l)-\frac{\pi}{2l_0^2}\sin[2\pi(q_l+f_l)]-f_l^{(1)}(X)\left[\ddot{X}+\frac{1}{2}\dot{X}^2\frac{d\ln M}{dX}\right]. \tag{3.7}$$

The coordinates q_l in Eq. (3.7) are coupled to the kink motion through $f_l^{(1)}$.

Equations (3.6) and (3.7) constitute a complete closed set of second-order differential equations for the N q's and X. The discreteness of the kink gives rise to q's which adiabatically "dress" its continuum form, as well as to radiated phonons when the kink is set in motion. Since the coupling between the kink and the q's is effected through $f_l^{(1)}=(1/l_0)\text{sech}[\pi(l-X)/l_0]$, the dominant instantaneous effect of the kink is on those q's which are within l_0 of the soliton coordinate.

IV. SPECIAL CASES

In Sec. III we derived the rigorous equations of motion for the N q_l's and X with no restrictions on the magnitudes of the dynamical variables or on the dimensionless parameter l_0. In order to elucidate the physical implications behind the above equations, we shall discuss in this section three important special cases. In the first case we consider the continuum limit, i.e., $l_0\gg 1$, where all q_l's approach zero. In this case, the only surviving equation of motion is Eq. (3.6), in which we have set $q_l=0$, i.e.,

$$\ddot{X}+\tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX}=(1/M)\sum_{l=1}^{N} f_l^{(1)}\left[f_{l+1}+f_{l-1}-2f_l-\frac{\pi}{2l_0^2}\sin(2\pi f_l)\right]$$
$$=\frac{2}{4!}\frac{1}{M}\sum_{l=1}^{N} f_l^{(1)}f_l^{(4)}+\frac{1}{M}\frac{2}{6!}\sum_{l=1}^{N} f_l^{(1)}f_l^{(6)}+\cdots\ , \tag{4.1a}$$

where we used

$$\frac{d^2f_l}{dl^2}=\frac{\pi}{2l_0^2}\sin(2\pi f_l) \tag{4.1b}$$

and

$$f_{l+1}-2f_l+f_{l-1}=\frac{d^2f_l}{dl^2}+\frac{2}{4!}\frac{d^4f_l}{dl^4}+\frac{2}{6!}\frac{d^6f_l}{dl^6}+\cdots\ . \tag{4.1c}$$

We can neglect the sixth derivative compared with the fourth when

$$\frac{2}{6!}\left[\frac{\pi}{l_0}\right]^6 \ll \frac{2}{4!}\left[\frac{\pi}{l_0}\right]^4 .$$

For example, for $l_0 \sim \pi$ the sixth-derivative term is approximately 3% of the fourth-derivative term. We can express Eq. (4.1) as

$$\ddot{X}+\tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dx}=-\frac{1}{M}\frac{dU}{dX}\ , \tag{4.2}$$

where

$$\frac{dU}{dX}=-\frac{2}{4!}\sum_{l=1}^{N} f_l^{(1)}f_l^{(4)}=\sum_{n=1}^{\infty} B_n\sin(2n\pi X)\approx B_1\sin(2\pi X)\ , \tag{4.3}$$

since

$$B_n=\frac{\pi^3 n^2}{3\sinh(n\pi l_0)}\left[2n^2+\frac{1}{l_0^2}\right] ,$$

as is shown in the Appendix. U is actually the Peierls-Nabarro potential. Several approximate estimates of its magnitude have been reported in the literature.[3–5,15–19] Equation (4.3) defines the bare form of this potential, which we will denote U_0^{PN}. The terms for $n>1$ decay rapidly as n increases because of the exponential functions in the denominator of B_n, so that the correction for $n=2$ is typically less than one part in 10^3 for $l_0 \sim \pi$ where the effects of discreteness are most important. The potential $U_0^{\mathrm{PN}}(X)$ can then be written

$$U_0^{\mathrm{PN}}(X)=U_0+\tfrac{1}{2}E_a\cos(2\pi X)\ , \tag{4.4}$$

where U_0 is a constant term and

$$E_a=\frac{B_1}{\pi}=\frac{\pi^2}{3\sinh(\pi l_0)}\left[2+\frac{1}{l_0^2}\right] .$$

Similarly the expression for the dimensionless mass M is

$$M\equiv\sum_{l=1}^{N}(f_l^{(1)})^2=\frac{2}{\pi l_0}+\sum_{n=1}^{\infty}A_n\cos(2\pi nX)\ , \tag{4.5}$$

where $A_n=4n[\sinh(n\pi l_0)]^{-1}$. Consequently, the X dependence of the mass is relatively unimportant and the constant value of the mass is inversely proportional to l_0 and goes to zero in the continuum limit $l_0\to\infty$. Further, since the X dependence of the mass is so weak the coefficient of the $\dot{X}^2$ term in Eq. (3.6), $d\ln M/dX$, is small and thus the $\dot{X}^2$ term can usually be neglected.

When we neglect the $\dot{X}^2$ term in Eq. (4.2), we obtain

$$\ddot{X}=-\frac{\omega_0^2}{2\pi}\sin(2\pi X)\ , \tag{4.6}$$

where

$$\omega_0^2\equiv-\frac{1}{M}\frac{\partial^2 U_0^{\mathrm{PN}}}{\partial X^2}\bigg|_{X=1/2}=\frac{2\pi}{M}B_1=\frac{\pi^5 l_0}{3\sinh(\pi l_0)}\left[2+\frac{1}{l_0^2}\right]$$

is the small-amplitude frequency of the soliton in the potential well. The well depth and ω_0^2 vanish exponentially as $l_0\to\infty$, i.e.,

$$E_a\sim\tfrac{4}{3}\pi^2 e^{-\pi l_0}\ \text{ as } l_0\to\infty \tag{4.7a}$$

and

$$\omega_0^2\sim\tfrac{2}{3}\pi^5 l_0 e^{-\pi l_0}\ \text{ as } l_0\to\infty\ . \tag{4.7b}$$

For $\pi=l_0$ we have $\omega_0\sim 0.18$ and the lowest frequency of the phonon spectra, namely π/l_0, is equal to unity. Thus, if a soliton was trapped oscillating at a frequency $\sim\omega_0$, it could radiate phonons only by a high-order parametric process. Consequently, a trapped soliton will behave almost like an undamped nonlinear oscillator.

Next we consider the case where $q\neq 0$ and the q_l's are generated by the presence of the soliton $f_l(X)$. When we linearize Eq. (3.7) for q_l, we obtain

$$\ddot{q}_l=q_{l+1}+q_{l-1}-2q_l-q_l\left[\frac{\pi}{l_0}\right]^2\cos(2\pi f_l)+f_{l+1}+f_{l-1}-2f_l-\frac{\pi}{2l_0^2}\sin(2\pi f_l)-f_l^{(1)}\left[\ddot{X}+\tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX}\right]$$
$$\approx q_{l+1}+q_{l-1}-2q_l-q_l\left[\frac{\pi}{l_0}\right]^2\cos(2\pi f_l)+\frac{2}{4!}f_l^{(4)}-f_l^{(1)}\left[\ddot{X}+\tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX}\right] , \tag{4.8}$$

where we used Eq. (4.1b) and the approximate equality follows from truncating Eq. (4.1c) at the fourth derivative. We introduce an N-dimensional vector notation where the components of the vector $\mathbf{q}$ are $(q_1, q_2, \ldots, q_N)$ and the components of the (column) vector $\mathbf{f}^{(1)}$ are $(f_1^{(1)}, f_2^{(1)}, \ldots, f_N^{(1)})^T$. Then Eq. (4.8) can be expressed in vector notation as

$$\ddot{\mathbf{q}} = \mathbf{A}\mathbf{q} + \frac{2}{4!}\mathbf{f}^{(4)} - \mathbf{f}^{(1)}\left[\ddot{X} + \tfrac{1}{2}\dot{X}^2 \frac{d\ln M}{dX}\right], \tag{4.9}$$

where the linear operator $\mathbf{A}$ is a tridiagonal matrix involving the $\mathbf{q}$ terms on the right-hand side of Eq. (4.8). In Ref. 19 we obtained the static solution for $\mathbf{q}$ in the presence of the kink. We have shown that the static solution $\mathbf{q}_s$ satisfies the equation

$$\mathbf{A}\mathbf{q}_s + \frac{2}{4!}\mathbf{f}^{(4)} - \lambda(X)\mathbf{f}^{(1)} = \mathbf{0}, \tag{4.10}$$

where the Lagrange multiplier λ is a function of X and is given explicitly in Ref. 19. The significant consequence of this approach is that exact results for $\mathbf{q}_s$, obtained by molecular-dynamics simulations, agree with the solution of the linear equation, Eq. (4.10), to within 1% or 2%. In a future publication[20] we will show that the spontaneous emission radiation of a single kink is also small and can be obtained from the linear equation (4.8).

We next express $\mathbf{q}(t)$ as the sum of two parts: one part is a dynamical dressing of the continuum kink $\mathbf{f}$ that follows $X(t)$ adiabatically and the second part represents phonons radiated by the kink as we will show later, i.e.,

$$\mathbf{q}(t) = \mathbf{q}_s(X(t)) + \delta\mathbf{q}(t). \tag{4.11}$$

We obtain an equation for the time dependence of $q_s(X(t))$ from Eq. (4.10) for the static $\mathbf{q}_s$ by the following argument. From Eq. (4.10) we can interpret $\lambda(X)f^{(1)}(X)$ as the external force that must be applied to cause $\ddot{\mathbf{q}}_s$ to vanish for a given position X of the soliton. We consider $\mathbf{q}_s(X(t))$ to be the static solution evaluated at the value X of the soliton at time t. Consequently, we have

$$\lambda(X(t))\mathbf{f}^{(1)}(X(t)) \equiv \ddot{\mathbf{q}}_s(X(t)) = \mathbf{A}\mathbf{q}_s(X(t)) + \frac{2}{4!}\mathbf{f}^{(4)}, \tag{4.12}$$

We obtain the equation of motion for $\delta\mathbf{q}(t)$ by substituting Eqs. (4.11) and (4.12) into Eq. (4.9), which becomes

$$\delta\ddot{\mathbf{q}} = \mathbf{A}\,\delta\mathbf{q} - \mathbf{f}^{(1)}\ddot{X} \approx \mathbf{A}\,\delta\mathbf{q} + \frac{1}{2\pi}\mathbf{f}^{(1)}\hat{\omega}^2\sin[2\pi X(t)], \tag{4.13}$$

where $\hat{\omega}^2$ is defined in Eq. (4.15). For convenience, we have neglected the small term $\mathbf{f}^{(1)}[\tfrac{1}{2}\dot{X}^2(d\ln M/dX)]$ in Eq. (4.13).

In Ref. 19 we found that the dependence of the potential V on q in the static kink case was, to a very good approximation, represented by a linear q dependence. In Ref. 20 we will show that the contribution of spontaneously emitted phonons can also be treated by assuming a linear dependence on q. Therefore, when we linearize the right-hand side of Eq. (3.6) with respect to q and substitute Eq. (4.11) in Eq. (3.7), we obtain

$$\ddot{X} + \tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX} = (1/M)\sum_{l=1}^{N} f_l^{(1)}\left[q_{l+1} + q_{l-1} - 2q_l - q_l\frac{\pi}{l_0^2}\cos(2\pi f_l) + \frac{2}{4!}f_l^{(4)}\right] \equiv -\frac{1}{M}\frac{dV_L}{dX}(X, \mathbf{q}_s + \mathbf{q}), \tag{4.14}$$

where the subscript L means V is linearized with respect to q. Starting with large l_0 and then decreasing l_0, we find a succession of three approximations for the equation of motion for the soliton coordinate $X(t)$. In the lowest approximation we have the bare Peierls-Nabarro limit Eq. (4.2). In next approximation we set $\delta\mathbf{q}$ equal to zero, and so that by using Eq. (4.10), we obtain

$$\ddot{X} + \tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX} = -\frac{1}{M}\frac{dV_L}{dX}(X, \mathbf{q}_s(X)) \equiv -\frac{1}{M}\frac{\partial U_D^{\mathrm{PN}}}{\partial X} \approx \frac{\hat{\omega}^2}{2\pi}\sin(2\pi X), \tag{4.15}$$

where U_D^{PD} is the dressed Peierls-Nabarro potential which results from the adiabatic dressing of the continuum kink $\mathbf{f}$ by the q's. U_D^{PN} retains the same functional dependence on X as U_0^{PN}, but its magnitude has been increased. This in turn leads to a renormalization of the frequency ω_0 in the Peierls-Nabarro well. The higher frequency results from a sharpening of the continuum kink f_l by the q_l leading to a sinusoidal potential for X with a higher curvature.

Finally, as will be demonstrated in Ref. 20, the $\delta\mathbf{q}$ dependence of V_L leads to spontaneously emitted phonons. The inclusion of $\delta\mathbf{q}$ results in an equation of motion for X of the form

$$\ddot{X} + \tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX} + \text{damping term} = -\frac{1}{M}\frac{dU_D^{\mathrm{PN}}}{dX}. \tag{4.16}$$

The damping term is obtained by first calculating the energy radiated by the kink, using Eq. (4.13) and then comparing the damping term with the calculated rate. The damping term is highly nonlinear and complicated. Except in the case of a very high-velocity regime, it cannot be represented by simple $\dot{X}$ or $\ddot{X}$ terms. For example, if the kink is trapped and oscillating in the PN potential, it can spontaneously emit only by a parametric process involving at least a cubic nonlinearity in X. The reason is that $\hat{\omega}_0$ is less than π/l_0, where π/l_0 is the lowest phonon frequency. It is necessary to have a frequency at least as large as $3\hat{\omega}_0$ to be in resonance with a lattice phonon. Thus, one of the consequences of the form of the damping term is that a kink trapped in the PN potential well will often oscillate with almost negligible damping.

V. COMPARISON WITH OTHER WORK

Although the question of discreteness effects has been addressed frequently in the past, to the best of our knowledge there have been very few attempts to develop a comprehensive formalism to describe the dynamic and the static properties of kinks in a discrete lattice. Ishimori and Munakata[5] have used a perturbative approach suggested by McLaughlin and Scott,[21] together with a Fourier decomposition of the structural perturbation source, to derive equations of motion for the kink and radiation. This approach has been successful in revealing several of the manifestations of discreteness. These authors were able to account qualitatively for the "wobbling" propagation of the kink center as well as the pinning due to the Peierls field. They have also calculated the magnitude of the bare PN barrier. Yet because of the complexity of the resulting equations, the ensuing analysis and interpretations were guided by mathematical convenience rather than by a clear physical picture. For example, the response to the constant source term in the Fourier decomposition was interpreted as the dynamical soliton dressing, while the remaining source terms led to radiative response. Since both the Green's function used and the constant term are translationally invariant with respect to the kink center, the resulting kink dressing is just a renormalization of the continuum form, still endowed with the manifestations of translational invariance. In contrast, the kink dressing that is treated within the present formalism incorporates the full granularity of the underlying space. Consequently, the dressing that results from our formalism is not limited to cases involving very "long" solitons.

Another approach is that of Combs and Yip,[4] who have attempted to adopt the field-theoretical variational approach of Tomboulis.[12] In essence, CY have employed a single constraint, namely C_1. Subsequently, they obtained an equation of motion for $\ddot{X}$ by differentiating the single constraint C_1 with respect to time and then using the original N equations of motion for $\ddot{Q}_l$ to obtain the equation of motion for $\ddot{X}$ which depends on the q_l. They have $N+1$ coordinates, namely the X and the q_l's, but they have not constructed, as we have done, a Hamiltonian system for $2(N+1)$ canonical variables. Instead, they used a mixed description, namely an equation of motion for X whose q_l dependence must be found from the original $2N$ Hamilton's equations for Q_l and P_l. Their equation for $\ddot{X}$, Eq. (3.10) of Ref. 4 can be written as

$$M_{\rm CY}\ddot{X}+\lambda\dot{X}+\zeta\dot{X}^2=-\frac{\partial V}{\partial X}\,, \tag{5.1}$$

where

$$M_{\rm CY}\equiv\sum_{l=1}^{N}[(f_l^{(1)})^2-f_l^{(2)}q_l]\,, \tag{5.2a}$$

$$\lambda\equiv-2\sum_{l=1}^{N}f_l^{(2)}\dot{q}_l\,, \tag{5.2b}$$

$$\zeta\equiv\sum_{l=1}^{N}(f_l^{(1)}f_l^{(2)}-f_l^{(3)}q_l)\,. \tag{5.2c}$$

It is immediately apparent from the above equations that the incomplete set of constraints employed in the CY approach leads to the dependence of the coefficients on the right-hand side of Eq. (5.1), namely $M_{\rm CY}$, λ, and ζ, on the q_l's. In contrast, in the present formulation the application of the two constraints C_1 and C_2 leads to the following: First, the expression for the mass M does not contain the term $\sum_l f_l^{(2)}q_l$ in Eq. (5.2a) and therefore depends solely on the $f_l^{(1)}$'s which, in turn, depend on l_0. Second, the coefficient λ vanishes, as we will show below. Third, the expression for the coefficient ζ does not contain the terms $\sum_l f_l^{(3)}q_l$ of Eq. (5.2c), and finally the q_l dependence of dV/dX in Eq. (5.1) is determined by our Eq. (3.7), which is not equivalent to Eq. (3.8) of Ref. 4. We shall now demonstrate why these terms of Eq. (5.1) vanish in our canonical formalism when both constraints C_1 and C_2 are invoked. We first multiply Eq. (3.7) by $f_l^{(1)}(X)$, sum over l, and use Eq. (3.6), resulting in $\sum_l f_l^{(1)}(X)\ddot{q}_l=0$. Next we differentiate C_2 with respect to t:

$$\frac{dC_2}{dt}=0=\sum_{l=1}^{N}f_l^{(1)}(X)\ddot{q}_l+\dot{X}\sum_{l=1}^{N}f_l^{(2)}(X)\dot{q}_l \sim 0+\dot{X}\sum_{l=1}^{N}f_l^{(2)}(X)\dot{q}_l\,. \tag{5.3}$$

Thus, as long as $\dot{X}\neq0$, Eq. (5.3) implies $\lambda=0$. If we differentiate C_1 with respect to t, we obtain

$$\frac{dC_1}{dt}=0=\sum_{l=1}^{N}f_l^{(1)}\dot{q}_l+\dot{X}\sum_{l=1}^{N}f_l^{(2)}q_l=0+\dot{X}\sum_{l=1}^{N}f_l^{(2)}q_l\,, \tag{5.4}$$

where $C_2=0$. Thus, as long as $\dot{X}\neq0$, Eq. (5.4) implies that $M_{\rm CY}=M$ because $\sum_l f_l^{(2)}q_l=0$. Finally, if we differentiate $\sum_l f_l^{(2)}q_l=0$ with respect to time, we obtain

$$\frac{d}{dt}\sum_{l=1}^{N}f_l^{(2)}q_l=0=\dot{X}\sum_{l=1}^{N}f_l^{(3)}q_l+\sum_{l=1}^{N}f_l^{(2)}\dot{q}_l =\dot{X}\sum_{l=1}^{N}f_l^{(3)}q_l+0\,, \tag{5.5}$$

where $\sum_l f_l^{(2)}\dot{q}_l=0$ because $dC_2/dt=0$ and $\sum_l f_l^{(1)}\ddot{q}_l=0$. Consequently, we see that the difference between the two equations for $\ddot{X}$ vanish when we use both constraints C_1 and C_2, and a full Hamiltonian theory for the $2N+2$ canonical coordinates is employed. The fact that the mass of the kink and the parameter ζ (which is proportional to $d\ln M/dX$) are independent of the q_l's is important for the following reason. Consider the case where a pulse of phonons $\sum_l c_l q_l$ is scattered off the kink. If M depended on the q_l's, the mass of the kink would be determined in part by the scattering pulse even when the pulse is spatially separated from the kink, instead of by the f_l's alone as in our Eq. (4.5). In Ref. 4 the authors have referred to the presence of $\lambda(t)$ in the context of a generalized Langevin equation. However, as we have shown above, $\lambda(t)$ vanishes. In Ref. 20 we will show that $X(t)$ does satisfy a highly nonlinear generalized Langevin equation by evaluating the radiation damping of the kink and using the fluctuation-dissipation theorem to obtain the proper fluctuation force.

Finally, the comparison that Combs and Yip have made between their equation for $\ddot{X}$ and the equivalent equations that result from the theories of Refs. 22–26 holds for our equations as well when the mass $M_{\rm CY}$ is set equal to M, λ is set equal to zero, and $\sum_l f_l^{(3)} q_l$ is set equal to zero in ξ. Further detailed discussions concerning each of the above points are given in Refs. 19 and 20, which are specifically devoted to addressing these questions.

IV. SUMMARY AND CONCLUSION

In this paper we have developed for the first time a rigorous Hamiltonian system of equations that introduces the coordinate of the kink center, X, and the N q_l's as $N+1$ canonical coordinates. With our Hamiltonian formalism we are able to treat, in a systematic manner, problems in which the discrete nature of the kinks dominates the physics of the manifest phenomena. We have outlined the procedure for introducing a nonperturbative static dressing $\mathbf{q}_s(X)$ to the bare (continuum) stationary soliton. In obtaining the static dressing solutions we have introduced for the first time the prescription for an external force that has the correct distribution among the chain particles to balance the Peierls forces and thus to leave the kink stationary, without distortions, at any position in the PN well. Subsequently, we have shown that this dressing can be transformed adiabatically to follow the motion of the center of the kink, namely $\mathbf{q}_s(X(t))$. The introduction of the dynamical dressing allows the separation of the purely radiative terms in $\mathbf{q}$, namely $\delta\mathbf{q}$. The details of each of these phenomena will be discussed and analyzed in separate publications,[19,20] in which the underlying physical subtleties are adequately exposed. In addition, we will evaluate the damping of the kink motion due to the spontaneous emission of phonons by solving the coupled equations, Eqs. (3.6) and (3.7), in a manner similar to the approach used in calculating radiation damping in electromagnetic theory, in a future publication. For the calculation of the spontaneous emission we will use the fact that the equation for $\delta\mathbf{q}$, Eq. (4.13), is linear in $\delta\mathbf{q}$. A second important problem that we will treat within the present formalism is the scattering of an external beam of phonons off a discrete kink using Eq. (4.14), where $\delta\mathbf{q}$ is determined by the external beam. The dominant term in the scattering is linear in $\delta\mathbf{q}$, in contrast to the continuum kink case where the scattering requires nonlinear terms in $\delta\mathbf{q}$. We will show that the scattering can be described in terms of scattering off a single particle, described by $X(t)$, which in the case of scattering from a periodic lattice of kinks will lead to umklapp processes. Finally, we would like to point out, that although we have confined our discussion to systems with a single kink, the procedure outlined in this paper can be generalized to include many kinks interacting with each other.

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APPENDIX

In the discrete problem we frequently have to evaluate functions having the general form

$$g(x)=\sum_{i=-\infty}^{+\infty} f(i-x)\ . \tag{A1}$$

This function is obviously periodic in x with period 1. Hence, we can expand it in a Fourier series

$$g(x)=\tfrac{1}{2}A_0+\sum_{n=0}^{\infty} A_n\cos(2n\pi x)+\sum_{n=0}^{\infty} B_n\sin(2n\pi x)\ . \tag{A2}$$

The coefficients of the series are given by

$$A_n=2\int_{-1/2}^{1/2}\sum_{i=-\infty}^{\infty} f(i-x)\cos(2n\pi x)dx\ . \tag{A3}$$

If we interchange the order of summation and integration and then change variables according to $z=i-x+1$, with a corresponding change in the limits of integration, we obtain

$$A_n=2\sum_{i=\infty}^{\infty}\int_{i-1/2}^{i+1/2} f(z)\cos[2n\pi(i-z)]dz\ . \tag{A4}$$

But

$$\cos[2n\pi(i-z)]=\cos(2n\pi z)\ ,$$

$$\sin[2n\pi(i-z)]=-\sin(2n\pi z)$$

and the integrand is independent of i. We can therefore evaluate the sum since it is just a sum of integrals of the same function over adjacent intervals:

$$A_n=2\int_{-\infty}^{\infty} f(z)\cos(2n\pi z)dz\ ,$$

$$B_n=-2\int_{-\infty}^{\infty} f(z)\sin(2n\pi z)dz\ . \tag{A5}$$

We notice from Eq. (A5) that $g(x)$ has the same parity as $f(x)$.

The expressions of the form of Eq. (A1) are those for dU/dX in Eq. (4.3) and the dimensionless mass in Eq. (4.5):

$$\frac{dU}{dX}=-\frac{2}{4!}\sum_{l=1}^{N} f_l^{(1)}f_l^{(4)}\ , \tag{4.3}$$

where, for example,

$$f_l^{(1)}=\frac{d}{dX}\frac{2}{\pi}\tan^{-1}(e^{\pi(l-X)/l_0})$$
$$=\frac{1}{l_0}\operatorname{sech}\left[\frac{\pi}{l_0}(l-X)\right] .$$

Since dU/dX is odd in X we can write

$$\frac{dU}{dX}=\sum_{n=1}^{\infty} B_n \sin(2n\pi X) , \quad \text{(A6)}$$

where from Eq. (A5),

$$B_n=\frac{1}{3!}\int_{-\infty}^{\infty} f^{(1)}(z)f^{(4)}(z)\sin(2n\pi z)dz . \quad \text{(A7)}$$

One integration by parts gives

$$B_n=\frac{-n\pi}{3}\int_{-\infty}^{\infty}[f^{(1)}f^{(3)}-\tfrac{1}{2}(f^{(2)})^2]\cos(2n\pi z)dz . \quad \text{(A8)}$$

Substituting the expressions for the derivatives we get

$$B_n=\frac{n\pi^3}{6l_0^4}\int_{-\infty}^{\infty}[3\operatorname{sech}^4(\pi z/l_0)-\operatorname{sech}^2(\pi z/l_0)] \times\cos(2n\pi z)dz . \quad \text{(A9)}$$

These integrals can be found in the tables, and after some algebraic manipulations the following result is obtained:

$$B_n=\frac{n^2\pi^3(2n^2-1/l_0^2)}{3\sinh(n\pi l_0)} . \quad \text{(A10)}$$

The mass is given by Eq. (4.5):

$$M(X)=\sum_{l=1}^{N}(f_l^{(1)})^2 . \quad \text{(4.5)}$$

The Fourier coefficients are then

$$A_n=\frac{2}{l_0^2}\int_{-\infty}^{\infty}\operatorname{sech}^2(\pi z/l_0)\cos(2n\pi z)dz , \quad \text{(A11)}$$

giving the final result

$$A_0=\frac{4}{\pi l_0}, \quad A_n=\frac{4n}{\sinh(n\pi l_0)} , \quad \text{(A12)}$$

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