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Effect of lattice discreteness on the statistical mechanics of a dilute gas of kinks

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We apply the collective-variable projection-operator approach based on the Dirac-bracket theory of constrained Hamiltonian systems to the calculation of the Helmholtz free energy of discrete nonlinear Klein-Gordon systems in the ideal-kink-gas limit. The kinks in the continuum nonlinear Klein-Gordon systems in the ideal-gas limit behave as free particles and the phonon density of states changes due to the presence of the kink. In discrete nonlinear Klein-Gordon systems the kinks are no longer free but see a potential $V_K(X)$ where X is the center of mass of the kink. The phonons satisfy the discrete-lattice dispersion law with a discrete density of states, which differs from the continuum density of states, which also changes in the presence of the discrete kink. We find that when l_0 (the effective size of the kink) is greater than about five lattice spacings that the effect of discreteness is to lower the rest energy of the kink by less than 1%. For $l_0 \sim \pi$ the rest energy of the kink is lowered further and the potential $V_K(X)$ starts to make a contribution giving rise to the presence of the periodic Peierls-Nabarro potential well. For $l_0 < \pi$ the Peierls-Nabarro well becomes deeper and the kinks start to become trapped and when $l_0 \leq 2$ all kinks with velocities less than one third of the speed of sound become trapped. In the strong-trapping region the rest energy of the kink is reduced by about 8–10%.

I. INTRODUCTION

The effect of discreteness on physical systems that are governed by equations of the nonlinear Klein-Gordon type, such as the sine-Gordon (SG), double sine-Gordon (DSG), and ϕ^4 equations, etc., range from small corrections of the continuum solutions to completely different phenomena which do not appear in the continuum. Examples of the latter case are trapping in the Peierls-Nabarro (PN) well, radiation from moving kinks in lattices,[1-3] and a host of phase transitions of the commensurate-incommensurate type.[4] A particularly important problem is the classical statistical mechanics of discrete nonlinear Klein-Gordon equations. Currie *et al.*[5] developed an ideal-gas phenomenology for continuum nonlinear Klein-Gordon equations based on the particlelike behavior of kinks at low temperatures where the density of kinks is low. They found agreement between the thermodynamic and static correlation functions obtained phenomenologically and the same quantities calculated by the exact transfer integral method. Recently Trullinger and Sasaki[6] examined the question of the effects of discreteness on the results of the transfer-operator method employed by Currie *et al.*[5] and obtained the lowest-order discreteness corrections to the continuum approximation of the transfer integral equation. Our purpose in this paper is to apply the Dirac-bracket theory of constrained Hamiltonian systems to the ideal-gas phenomenology of nonlinear Klein-Gordon systems. Our formalism is valid for the case where the kink size is as small as one or two lattice spacings where the effects of discreteness are so large that the trapping of the kink in the PN potential well plays an important role. For convenience in presentation we will treat explicitly the case of the discrete SG kink although the present approach applies to the discrete DSG, ϕ^4, or any other kink-bearing system.

In discrete nonlinear Klein-Gordon theories the energy of the kink depends on location of its center of mass. In continuum theories it does not unless perturbing potentials are present. In either case it is useful to exploit the particlelike nature of the kink by representing the location of its center of mass by the collective variable X. One of the advantages of a Hamiltonian collective-variable theory is that the parameter X is promoted to being a canonical variable with conjugate momentum P_X. In the continuum case X is cyclic and the Hamiltonian depends only on P_X. However, in discrete nonlinear Klein-Gordon theories the collective variable X moves in a nonconstant potential $V(X)$ which we obtain in Sec. II.

In a series of recent papers we have investigated the effects of discreteness on nonlinear Klein-Gordon equations using the projection-operator approach to collective variables which we have shown to be rigorously equivalent to the Dirac-bracket theory of constrained Hamiltonian systems.[7] We used this approach to derive the exact equations of motion for the center of mass X of a discrete SG kink and the frequency of its small oscillations $\omega_{\rm PN}$ in the PN well[8] and obtained essentially exact agreement with simulations. We have also[3] calculated the spontaneous emission of radiation from a discrete SG kink and obtained remarkable agreement with simulations. We found that a trapped kink radiates phonons very slowly (with a power-law decay rate) except for several phonon bursts which are emitted by the kink when an harmonic of the PN frequency passes into the phonon continuum which permits that harmonic to resonate with phonon states thereby producing radiation. The average energy loss per cycle is typically less than 0.1%. For the untrapped case, the radiation rate is deter-

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mined by harmonics of the frequency $2\pi v$ (v is the dimensionless ratio of the velocity of the particle to the speed of sound). The radiation rate decreases discontinuously when an harmonic of $2\pi v$ passes out of the phonon band and can no longer radiate phonons. The kink therefore loses energy until it becomes trapped. For the purpose of the present paper we note that the radiation rates for untrapped kinks are greater than the radiation rates for trapped kinks but still are small except for kinks moving near the speed of sound. The radiation rates in all cases go to zero for $l_0 \gg \pi$ experimentally as $\exp(-\pi l_0)$ where $2\pi/l_0$ is the slope of the kink at its center and l_0 is a rough measure of the size of the kink. Therefore, since we consider a nonrelativistic dilute gas of kinks in the present paper, we are able to neglect radiation effects.

An important physical manifestation of discreteness with which we shall be concerned in the present paper is the modification of the continuum kink energy. We show below that discreteness not only superimposes a periodic modulation on the continuum energy but also lowers the dc value. We will refer to the lowering of the dc value as the X-independent discreteness correction to the kink energy.

The relative importance of the X dependence of $V(X)$ in the dilute-kink-gas phenomenology depends crucially on the size of the kink l_0. In our units (which we will define in the next section) we find that for $l_0 \gg \pi$ the X dependence vanishes as $\exp(-\pi l_0)$. For $l_0 \sim \pi$ the explicit X dependence of the PN well contributes only about 2–4 % of the shift in the kink rest energy due to discreteness, and for $l_0 < \pi$ the X dependence is responsible for trapping the kinks with nonrelativistic velocities in the PN well and thus dominates the discreteness effect's contribution to the system's free energy.

We obtain in the limit $l_0 \gg \pi$ the result of Ref. 6 in which the X-independent lattice discreteness corrections in the transfer method for kink-bearing chains was evaluated. For $l_0 > \pi$ we use a perturbation theory developed in Ref. 9 for discrete kink systems to calculate analytically the X-dependent contributions to the free energy. For $l_0 \le \pi$ where we do not have analytic expressions for the X-dependent contribution, we obtain the necessary information from simulation. For $l_0 \sim 2$ where discreteness effects are relatively large we find that the bottom of the PN well is about 8–10 % below the creation energy of the continuum SG kink, and consequently the probability of creating a kink is increased by about the same factor.

In Sec. II we obtain the discrete SG Hamiltonian in terms of the collective variables. We obtain the Helmholtz free energy of the dilute gas of SG kinks in Sec. III. In Sec. IV we evaluate the free energy using a perturbation theory that treats the discreteness as a small perturbation. We evaluate the free energy nonperturbatively in Sec. V and discuss our results in Sec. VI.

II. HAMILTONIAN FOR THE DISCRETE SINE-GORDON EQUATION

The Hamiltonian for the discrete SG equation[7]

$$\ddot{Q}_l - \Delta_2 Q_l + \left[\frac{\pi}{l_0}\right]^2 \sin Q_l = 0 , \qquad (2.1)$$

where $\Delta_2 h_l \equiv h_{l+1} + h_{l-1} - 2h_l$ is

$$H = \tfrac{1}{2}\sum_i P_i^2 + \tfrac{1}{2}\sum_i (Q_{i+1} - Q_i)^2 + \left[\frac{\pi}{l_0}\right]^2 \sum_i (1 - \cos Q_i) , \qquad (2.2)$$

where $P_i = \dot{Q}_i$ and Q_l is the displacement of the lth particle from the lth substrate potential well in units of the substrate wavelength. The Hamiltonian in terms of collective variables X, P, q_l, and p_l defined by

$$Q_l(X(t),t) = \hat{f}_l(X(t)) + q_l(t) \qquad (2.3)$$

is

$$H = \frac{P^2}{2M(X)[1-b(X)]^2} + \tfrac{1}{2}\sum_i p_i^2 + V(X) , \qquad (2.4a)$$

where

$$V(X) = \tfrac{1}{2}\sum_i (\hat{f}_{i+1} - \hat{f}_i + q_{i+1} - q_i)^2 + \left[\frac{\pi}{l_0}\right]^2 \sum_i [1 - \cos(\hat{f}_i + q_i)] , \qquad (2.4b)$$

and where

$$b(X) \equiv \frac{1}{M(X)} \sum_j \hat{f}_j'' q_j \qquad (2.4c)$$

and

$$M(X) = \sum_j (\hat{f}_j')^2 . \qquad (2.4d)$$

The prime denotes the derivative with respect to the argument. The definition of the displacement $\hat{f}_i$ is[8]

$$\hat{f}_i(X(t)) = f_i(\tfrac{1}{2}) + \int_{1/2}^{1-X(t)} \psi_i(X'(t'))dX' , \qquad (2.5a)$$

where $f_i(\frac{1}{2})$ is the exact ground state of the discrete SG system ($X=\frac{1}{2}$ at the bottom of the PN well) and satisfies

$$f_{i+1} + f_{i-1} - 2f_i - \left[\frac{\pi}{l_0}\right]^2 \sin f_i = 0 \qquad (2.5b)$$

and ψ_i is the solution of the following equation:[8]

$$\left[\frac{\pi}{l_0}\right]^2 \psi_i(X)\cos f_i(X) - \Delta_2 \psi_i(X) = \omega^2(X)\psi_i(X) - \alpha(X)\psi_i(X) . \qquad (2.5c)$$

$\alpha(X)$ is a Lagrange multiplier and $\alpha(X)\psi_i(X)$ is the force needed to hold the kink at X. When $X=\frac{1}{2}$ then $\alpha(\frac{1}{2})=0$ and Eq. (2.5c) becomes the eigenvalue equation

$$\left[\frac{\pi}{l_0}\right]^2 \psi_i(\tfrac{1}{2})\cos f_i(\tfrac{1}{2}) - \Delta_2 \psi_i(\tfrac{1}{2}) = \omega_b^2 \psi_i(\tfrac{1}{2}) , \qquad (2.5d)$$

where ω_b^2 is the lowest eigenvalue of the excitations above the ground state. Equation (2.5d) is Eq. (2.1) linearized about the exact ground-state solution $f_i(\frac{1}{2})$. As $l_0 \gg \pi$, $\psi_i(\frac{1}{2})$ becomes the Goldstone mode of the continuum SG and $\omega_b \to 0$. ω_b is the PN frequency of the small oscillation of the kink about $X=\frac{1}{2}$. The q_l in Eq. (2.3) represent the functions which must be added to $\hat{f}_l$ in order to obtain the exact dynamical solution Q_l.

The introduction of collective variables for the kink (X and its conjugate momentum P) increases the number of degrees of freedom of the system by two. To conserve the number of degrees of freedom of the original system (Q_i,P_i) we need to specify two constraints and they are

$$C_1 \equiv \sum_i \hat{f}_i'(X) q_i(t)=0, \quad C_2 \equiv \sum_i \hat{f}_i'(X) p_i(t)=0 , \tag{2.6}$$

where p_i is the momentum conjugate to q_i and the prime denotes the derivative with respect to the argument. For the proof and a full discussion of the equivalence between the Hamiltonian equations of motion for $\dot{Q}_i$ and $\dot{P}_i$ from Eq. (2.2) and the collective-variable equations of motion for $\dot{X}$, $\dot{P}$, $\dot{q}_i$, and $\dot{p}_i$ from Eq. (2.4a) see Ref. 7. Also see Ref. 8 for a complete discussion of the function $\hat{f}_i$, calculation of the PN frequency $\omega_{\rm PN}$, and an analysis of various perturbation approaches to the discrete SG system and their dependence on l_0. In the preceding equations and the rest of the present paper we are using dimensionless units[8] $Q_i=2\pi x_i/a$, x_i is the displacement of the ith particle from the ith trough of the substrate potential, a is the period of the substrate potential, the dimensionless time is $\tau \equiv t\sqrt{\mu/m}$ where μ is the force constant of the springs, m is the mass of a single particle, and the effective coupling constant l_0 (which is a measure of the size of the kink) is given by $l_0^2 \equiv \mu a^2/(2W)$ where $W/2$ is the amplitude of the substrate potential.

In the ideal-gas phenomenology of SG kinks we treat the phonons to second order so on expanding Eq. (2.4b) to second order in q_i we obtain

$$V^{(2)}(X)=V_K+V_p^{(2)}+V_{\rm int} , \tag{2.7a}$$

where

$$V_K \equiv \tfrac{1}{2}\sum_i (\hat{f}_{i+1}-\hat{f}_i)^2+\left[\frac{\pi}{l_0}\right]^2 \sum_i (1-\cos\hat{f}_i) , \tag{2.7b}$$

$$V_p^{(2)} \equiv \tfrac{1}{2}\sum_i \left[(q_{i+1}-q_i)^2+\left[\frac{\pi}{l_0}\right]^2 q_i^2 \cos\hat{f}_i\right] , \tag{2.7c}$$

$$V_{\rm int} \equiv \sum_i \left[(\hat{f}_{i+1}-\hat{f}_i)(q_{i+1}-q_i)+\left[\frac{\pi}{l_0}\right]^2 q_i \sin\hat{f}_i\right] . \tag{2.7d}$$

The replacement of $V(X)$ by $V^{(2)}$ assumes the anharmonic interaction between phonons is negligible. We want to keep V_K to all orders in π/l_0 so that we can include nonlinear oscillations and trapping in the PN well. The ansatz $V^{(2)}$ for V is reasonable because as we shall show the energy changes due to discreteness are a small correction to the rest energy of the kink.

III. HELMHOLTZ FREE ENERGY OF THE DILUTE GAS OF SG KINKS

Currie *et al.*[5] derived the expression for the grand canonical partition function Ξ for the dilute-gas kink system as a function of Z_1, the partition function for the single-kink sector, and Z_0, the partition function for the zero-kink sector. Their result is

$$\Xi = Z_0 \exp(2e^{\beta\mu}\mathcal{Z}_1) , \tag{3.1}$$

where $\mathcal{Z}_1 \equiv Z_1/Z_0$. The factor of 2 arises from kink and antikink contributions. μ is the chemical potential which we can set equal to zero for the case (which we are considering) where the period of the substrate is the same as the period of the elastic chain; $\beta \equiv (kT)^{-1}$. The free energy G is

$$G \equiv -kT\ln\Xi = G_0 - 2kT\mathcal{Z}_1 . \tag{3.2}$$

G_0 is the free energy of the phonons in the absence of any kinks. When we divide Eq. (3.2) by the length L of the system we obtain

$$g=g_0-kT\langle n\rangle \quad \text{where } \langle n\rangle \equiv 2\mathcal{Z}_1/L \tag{3.3}$$

and $\langle n\rangle$ is the density of kinks and antikinks. Currie *et al.*[5] showed that the low-temperature statistical mechanics of continuous nonlinear Klein-Gordon kink systems required knowledge of interactions between the excitations of the nonlinear Hamiltonian. The required knowledge was shown to reside in the phase shift function $\Delta(k)$ which for the continuous SG is

$$\Delta_c(k)=\pi\frac{k}{|k|}-2\tan^{-1}\left[\frac{kl_0}{\pi}\right] . \tag{3.4}$$

Their result[5] for $\langle n\rangle_c$ (where the c denotes the continuum) in our units is

$$\langle n\rangle_c=\frac{1}{\sqrt{2\pi}}\left[\frac{2\pi e^{\sigma_c}}{l_0}\right](\beta E_K^0)^{1/2}\exp(-\beta E_K^0) , \tag{3.5a}$$

where $E_K^0=8\pi/l_0$ is the rest energy of the kink and[5]

$$\sigma_c \equiv -\frac{1}{2\pi}\int_{0+}^{\infty} dk \frac{d\Delta_c}{dk}\ln\left[1+\left[\frac{l_0 k}{\pi}\right]^2\right] . \tag{3.5b}$$

The form of Eq. (3.5b) is a consequence of the dispersion law of the continuum SG equation

$$\omega^2(k)=\left[\frac{\pi}{l_0}\right]^2+k^2 . \tag{3.6}$$

(Note the speed of sound is one in our units.) The form of Eq. (3.5a) with Eq. (3.5b) follows from the fact that the frequency dispersion law is the same in the absence of the kink as in the presence of the kink and the only net effect in the statistical mechanics is a change in the density of states $\Delta_c(k)$ of the phonons between the cases where the kink is absent, Z_0, and the case where a kink is present, Z_1. As long as the dispersion law in the discrete case is the same in the absence of the kink as in the presence of the kink (and if there are no other direct interactions between phonons and kinks) we will be able to obtain the same expression $\exp(\sigma_d)$ for the phonon contribution where now σ_d depends on discrete dispersion law

$$\omega^2(k)=\left[\frac{\pi}{l_0}\right]^2+4\sin^2\left[\frac{k}{2}\right] \tag{3.7}$$

and $\Delta_c(k)$ in Eq. (3.5b) is replaced by the phase shift $\Delta_d(k)$ of the discrete SG.

We have shown[10] the collective-variable approach for the center of mass variable X and P for the continuum SG gives exactly the same result as Eqs. (3.5a) and (3.5b). In order to calculate the free energy of the discrete kink-antikink gas we need to calculate Z_1 (the partition function in the single-kink sector) in the dilute-kink limit, i.e.,

$$Z_1=\int e^{-\beta H^{(2)}}\delta\left[\sum_j \hat{f}'_j q_j\right]\delta\left[\sum_j \hat{f}'_j p_j\right]dX\,dP \times\prod_i dq_i dp_i\ , \tag{3.8}$$

where $H^{(2)}$ is obtained from H, Eq. (2.4a), by replacing $V(X)$, Eq. (2.4b), by $V^{(2)}(X)$ given by Eq. (2.7a). The only effect of the constraints in Eq. (3.8) is to cause the variables q_i and p_i to be expressed as linear combinations of only the phonon normal modes which are given by the nonlocalized eigenfunctions of Eq. (2.5d), i.e., the q_i and p_i have no component in the $\hat{f}'_j$ direction. Denoting the components by $q_{(1)}\equiv C_1$ and $p_{(1)}\equiv C_2$, where C_1 and C_2 are defined in Eq. (2.6), we have $q_{(1)}=p_{(1)}=0$ and the corresponding eigenfrequency is $\omega_{(1)}=\omega_{\rm PN}$.

The P integration in Eq. (3.8) is

$$\int_{-\infty}^{\infty}dP\exp\left[-\frac{\beta}{2}\frac{P^2}{M(X)[1-b(X)]^2}\right]=\left[\frac{M(X)2\pi}{\beta}\right]^{1/2}[1-b(X)]\ . \tag{3.9}$$

In the case where $V_p^{(2)}$ is an even function of q_i, we find that $\langle b(X)\rangle$ averaged over the q_i's vanishes and the integral over P in Eq. (3.9) is $[2\pi M(X)kT]^{1/2}$. Furthermore, if $V_{\rm int}$ in Eq. (2.7a) vanishes or is negligible then when we divide Z_1 by Z_0 the integral over the phonon coordinate in Z_1 is the same as the integral Z_0 except for the fact that the density of states is different in the two integrals due to the presence of the kink. Thus the collective-variable approach[10] gives the same factor e^{σ} as was first obtained by Currie *et al.*[5] in the continuum case except their σ_c, Eq. (3.5b) is replaced by σ_d where

$$\sigma_d\equiv-\frac{1}{2\pi}\int_{0+}^{\infty}dk\frac{d\Delta_d(k)}{dk}\times\ln\left[1+\left[\frac{l_0}{\pi}\right]^2 4\sin^2\left[\frac{k}{2}\right]\right]\ , \tag{3.10}$$

where $\Delta_d(k)$ is the phase shift in the discrete SG equation, whose properties were determined in Ref. 11. They found three ranges of behavior: (1) for $ka\ll 1$, $\Delta_d(k)\approx\Delta_c(k)$; (2) for intermediate values of k the discrete SG is reflectionless but $\Delta_d(k)$ differs quantitatively from $\Delta_c(k)$; and (3) for $|ka-\pi|\ll 1$ the Brillouin-zone edge in the discrete SG is no longer reflectionless but $\Delta_d(k)$ can be obtained analytically.

Consequently when we combine Eqs. (3.3), (3.5a), (3.8), (3.9), and (3.10) we obtain

$$\langle n\rangle_d=\langle\hat{n}\rangle_c\frac{1}{L}\int_0^L dX\left[\frac{M(X)}{E_K^0}\right]^{1/2}e^{-\beta[V_K(X)-E_K^0]}\ , \tag{3.11}$$

where $\langle\hat{n}\rangle_c$ is the density of kinks and antikinks in the continuum SG case Eq. (3.5a) with σ_c Eq. (3.5b) replaced by σ_d Eq. (3.10). In the limit $l_0\gg\pi$, $V_K(X)\rightarrow E_K^0$, $M(X)\rightarrow E_K^0$, and $\sigma_d\rightarrow\sigma_c$ and thus the discrete SG approaches the continuum SG result. We show in the next section that $M(X)$ differs very little from E_K^0. As a result the discreteness enters in essentially two places, σ_d and the X integration in Eq. (3.11). In the next section we investigate Eq. (3.11) using perturbation theory, i.e., the limit where $l_0\gg\pi$.

IV. PERTURBATION THEORY FOR THE DISCRETE SINE-GORDON SYSTEM

In the region $l_0\le\pi$ where discreteness effects are most important we do not have analytic solutions for the discrete SG and we have to resort to numerical methods or simulations as we do in the next section. In the near continuum region where $l_0>\pi$ the effects of discreteness are smaller but they make observable corrections to the continuum theory. Fortunately we can calculate the corrections analytically.[9] In order to motivate the perturbation theory we consider the equations of motion for $\ddot{X}$ derived in Refs. 7 and 9:

$$\ddot{X}=-\frac{1}{M}\sum_n\bar{f}'_n\left[\ddot{q}_n+\dot{X}^2\bar{f}''_n+\frac{\partial V(X)}{\partial q_n}\right]\ , \tag{4.1}$$

where $V(X)$ is given by Eq. (2.4b) and $\bar{f}_n(X)=4\tan^{-1}\{\exp[\pi(n-X)/l_0]\}$ (which is the soliton solution of the continuum SG evaluated at the lattice points). When we set in Eq. (4.1) all $q_n=0$ we obtain

$$\ddot{X}+\tfrac{1}{2}\dot{X}^2\frac{d\ln M}{dX}=\frac{1}{M}\sum_n\bar{f}'_n\left[\Delta_2\bar{f}_n-\left[\frac{\pi}{l_0}\right]^2\sin\bar{f}_n\right]=\frac{2}{4!}\frac{1}{M}\sum_n\bar{f}_n^{(1)}\bar{f}_n^{(4)}+\frac{2}{6!}\frac{1}{M}\sum_n\bar{f}_n^{(1)}\bar{f}_n^{(6)}+\cdots\equiv-\frac{1}{M}\frac{dU}{dX}\ , \tag{4.2a}$$

where we used

$$\frac{d^2\bar{f}_n}{dn^2}=\left[\frac{\pi}{l_0}\right]^2\sin\bar{f}_n\ , \tag{4.2b}$$

$$\Delta_2\bar{f}_n=\bar{f}_{n+1}+\bar{f}_{n-1}-2\bar{f}_n=\frac{d^2\bar{f}_n}{dn^2}+\frac{2}{4!}\frac{d^4\bar{f}_n}{dn^4}+\frac{2}{6!}\frac{d^6\bar{f}_n}{dn^6}+\cdots\ , \tag{4.2c}$$

and the notation $\bar{f}_n^{(i)}$ indicates $d^i\bar{f}_n(X)/dX^i$. [The function $\bar{f}_n(X)$ of the present paper is 2π times the f_n of Refs. 7 and 9.] Our perturbation theory consists of keeping only the terms $\bar{f}_n^{(2)}$ and $(2/4!)\bar{f}_n^{(4)}$ on the right-hand side of Eqs. (4.2a) and (4.2c) which is effectively an expansion in $(\pi/l_0)^2$ since each succeeding term is a factor of $(\pi/l_0)^2$ smaller. Thus the lowest-order term on the right-hand side of Eq. (4.2a) is[9]

$$\frac{dU}{dX}=-\frac{2}{4!}\sum_n \bar{f}_n^{(1)}\bar{f}_n^{(4)}=\sum_n B_n\sin(2\pi nX)\ , \tag{4.3}$$

where

$$B_n=-\frac{4\pi^5 n^2}{3\sinh(n\pi l_0)}\left[2n^2+\frac{1}{l_0^2}\right]\ , \tag{4.4}$$

where we used the fact that the potential U is periodic in X and we evaluated the coefficients B_n in the Fourier series. [Note Eq. (4.4) includes a minus sign correcting the expression for B_n which appears just below Eq. (4.3) of Ref. 9(a).] Consequently, the potential $U(X)$ is

$$U(X)=E_K^0+U_0+\sum_{n=1} C_n[1-\cos(2\pi nX)]\ , \tag{4.5a}$$

where

$$C_n=\frac{B_n}{2\pi n}=-\frac{2\pi^4 n}{3\sinh(n\pi l_0)}\left[2n^2+\frac{1}{l_0^2}\right]\ . \tag{4.5b}$$

According to Eq. (4.5a) the crests of the periodic PN barrier are positioned at $X=n$ where $n=0,\pm1,\pm2.\ldots$ In order to evaluate U_0 in the limit $l_0\gg\pi$ we approximate V_K given by Eq. (2.7b) by replacing $\hat{f}_i$ by $\bar{f}_i$ to obtain

$$\begin{aligned}\bar{V}_K&=\tfrac{1}{2}\sum_i(\bar{f}_{i+1}-\bar{f}_i)^2+\left[\frac{\pi}{l_0}\right]^2\sum_i(1-\cos\bar{f}_i)\\&=\tfrac{1}{2}\sum_i\bar{f}_i(2\bar{f}_i-\bar{f}_{i+1}-\bar{f}_{i-1})+\tfrac{1}{2}\sum_i(\bar{f}_i')^2\ ,\end{aligned}$$

where the second equality is obtained by shifting indices in the first term and replacing the second term by using

$$\tfrac{1}{2}\sum_i(\bar{f}_i')^2=\left[\frac{\pi}{l_0}\right]^2\sum_i(1-\cos\bar{f}_i)\ . \tag{4.5c}$$

We obtained Eq. (4.5c) by integrating Eq. (4.2b) and applying the boundary conditions $\bar{f}_i'\to0$ as $i\to\pm\infty$. Expanding the second difference using Eq. (4.2c), retaining up to and including fourth-derivative terms, and converting sums to integrals with $\bar{f}_i\to\bar{f}(x)$ we obtain

$$\bar{V}_K\approx-\tfrac{1}{2}\int dx\,\bar{f}\left[\frac{2}{2!}\frac{d^2\bar{f}}{dx^2}+\frac{2}{4!}\frac{d^4\bar{f}}{dx^4}\right]+\tfrac{1}{2}\int dx(\bar{f}')^2 \tag{4.5d}$$

and so

$$\bar{V}_K=E_K^0-\frac{1}{72}\left[\frac{\pi}{l_0}\right]E_K^0+X\text{-dependent terms}\ . \tag{4.5e}$$

For $l_0\gg\pi$ the coefficients of the X-dependent terms in Eqs. (4.5a) and (4.5e) go to zero as $\exp(-n\pi l_0)$ and therefore we make the identification

$$\begin{aligned}U_0&=-\frac{1}{2}\frac{2}{4!}\int\left[\frac{d^2\bar{f}_n}{dn^2}\right]^2dn\\&=-\frac{1}{9}\left[\frac{\pi}{l_0}\right]^3=-\frac{1}{72}\left[\frac{\pi}{l_0}\right]^2E_K^0\ .\end{aligned} \tag{4.5f}$$

The energy shift U_0 is the amount the kink rest energy is lowered below the continuum rest energy of the kink, i.e., it is the X-independent kink-rest-energy shift. U_0 is the same lowering of the kink rest energy as was obtained in Refs. 6 and 2. The kink rest energy E_K^0 results from integrating first and last terms in Eq. (4.5d) and U_0 arises from integrating the second term Eq. (4.5d). Equation (4.5a) for $U(X)$ is V_K of Eq. (2.7b) evaluated to the first-order correction to the continuum, i.e., replacing the left-hand side of Eq. (4.2c) by the first two terms on the right-hand side of Eq. (4.2c). $E_K^0[1-(\pi/l_0)^2/72]$ is the energy of the top of the PN barrier, in the limit $l_0\gg\pi$, i.e., for $l_0=4$ we obtain $U_0=-0.0554$ from simulation and $U_0=-0.0538$ from Eq. (4.5f) which gives an error of 2.9%. As l_0 becomes large the PN well vanishes leaving only a dc shift in the kink energy. The analytic expression for U_0 approaches the simulation value slowly, i.e., for $l_0=8$ (where simulation shows that the PN well has essentially disappeared and only the dc shift remains) we find U_0 differs from the simulation dc shift by as much as 1%.

Next we evaluate $V_p^{(2)}$ to the same order by using the first two terms of the identity Eq. (4.2c) in Eq. (2.7c) for the finite difference term $\sum_i(q_{i+1}-q_i)^2$. The result is

$$V_p^{(2)}\to\tfrac{1}{2}\sum\Omega_k^2q_{(k)}^2\ , \tag{4.6}$$

where the $q_{(k)}$ are the phonon normal modes in the absence of the kink. The frequency Ω_k is

$$\begin{aligned}\Omega_k&=\left[\left[\frac{\pi}{l_0}\right]^2+k^2+\frac{k^4}{12}\right]^{1/2}\\&=\left[\frac{\pi}{l_0}\right]\left[1+\tilde{k}^2+\left[\frac{\pi}{l_0}\right]^2\frac{\tilde{k}^4}{12}\right]^{1/2}\ ,\end{aligned} \tag{4.7}$$

where $\tilde{k}\equiv k(l_0/\pi)$ and since in our units $a=1$ the usual term $(ka)^2$, etc. just becomes k^2. Equation (4.7) without the k^4 term is just the dispersion law for the continuum which comes from the first term on the right-hand side of Eq. (4.2c). The second term of Eq. (4.2b), the fourth-derivative term is responsible for the k^4 term. The expansion of the dispersion law for the discrete harmonic lattice, Eq. (3.7), to k^4 gives exactly Eq. (4.7). Consequently, to first order in the discreteness correction, it is consistent to replace Eq. (4.7) by Eq. (3.7). We find that in the continuum limit V_{int}, Eq. (2.7d) vanishes. The first-order correction due to discreteness does not vanish and is linear in the q_i's which means the phonon potential energy is centered not on zero but on a value shifted by the presence of the kink. However, the final contribution of V_{int} to the free energy per particle is proportional to $\exp[\frac{1}{4}(2/4!)^2(\pi/l_0)^2I_f]$ where I_f is an integral of $\bar{f}_n^{(2)}$ over the eigenfunction of the linearized continuum SG operator which can be carried out analytically. However, the term in square brackets is always less than 10^{-3} in the range of validity of our perturbation theory, i.e., $l_0 \gg \pi$ and thus $V_{\rm int}$ can be neglected in our perturbation theory about the continuum. Consequently, the phonon contribution to the free energy is $\exp(\sigma_d)$ where σ_d is given by Eq. (3.10).

In the expression for C_n, Eq. (4.5b), we see that $C_n \sim \exp(-n\pi l_0)$ and thus the C_n decay very rapidly with n, therefore it is sufficient to keep the first term C_1, and thus the expression for V_K becomes

$$V_K(X)=E_K^0+U_0+\frac{\Delta_{\rm PN}}{2}[\cos(2\pi X)-1] , \tag{4.8}$$

where $\Delta_{\rm PN}/2=|C_1|$ and $\Delta_{\rm PN}=2M_0(\omega_{\rm PN}/2\pi)^2$ is the depth of the PN well. In our units $M_0=E_K^0$ because the speed of sound is equal to one. We can express our perturbation theory result for $V_K(X)$ as

$$V_K(X)=E_K^0\left[1-\frac{1}{72}\left[\frac{\pi}{l_0}\right]^2-\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2+\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\cos(2\pi X)\right] . \tag{4.9}$$

When we substitute Eq. (4.9) for $V_K(X)$ in Eq. (3.11) for $V(X)$ we obtain

$$\begin{aligned}\langle n\rangle_d&=\langle \hat n\rangle_c \exp\left\{\beta E_K^0\left[\frac{1}{72}\left[\frac{\pi}{l_0}\right]^2+\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\right]\right\}\frac{1}{L}\int_0^L dX\left[\frac{M(X)}{M_0}\right]^{1/2}\exp\left[-\beta E_K^0\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\cos(2\pi X)\right]\\
&=\langle \hat n\rangle_c \exp\left\{\beta E_K^0\left[\frac{1}{72}\left[\frac{\pi}{l_0}\right]^2+\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\right]\right\} I_0\left[\beta E_K^0\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\right]\left[1+\frac{\Delta M}{M_0}\frac{\partial \ln I_0}{\partial\left[\beta E_K^0\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\right]}\right] ,\end{aligned} \tag{4.10}$$

where I_0 is the modified Bessel function. The term proportional to $\Delta M/M_0$ is due to the X dependence of the mass where

$$\begin{aligned}\left[\frac{M(X)}{M_0}\right]^{1/2}&=\left[1+\frac{\sum_{n=1} A_n\cos(2\pi nX)}{M_0}\right]^{1/2}\\
&\approx\left[1+\frac{A_1}{M_0}\cos(2\pi X)\right]^{1/2}\\
&\approx 1+\frac{\Delta M}{M_0}\cos(2\pi X)\end{aligned} \tag{4.11}$$

with

$$\frac{\Delta M}{M_0}\equiv\frac{A_1}{2M_0} \quad\text{and}\quad \frac{A_n}{M_0}=\frac{2\pi n l_0}{\sinh(n\pi l_0)} .$$

Since the term $\Delta M/M_0 \approx 0.002$ for $l_0=4$, we see that the X dependence of the M is negligible and we can set $[M(X)/M_0]^{1/2}$ equal to one in Eq. (4.10). Furthermore, at $l_0=4$, $\omega_{\rm PN}/(2\pi)$ is 1.18×10^{-4} so that the modified Bessel function is $I_0[\beta E_K^0(1.4\times 10^{-4})]\approx 1$ for reasonable values of the parameter βE_K^0. (The parameter βE_K^0 has to satisfy the condition $\beta E_K^0 \gg 1$ to justify the dilute-kink approximation). Finally we find that

$$\langle n\rangle_d=\langle \tilde n\rangle_c \exp\left\{\beta E_K^0\left[\frac{1}{72}\left[\frac{\pi}{l_0}\right]^2+\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\right]\right\} \tag{4.12}$$

for the first-order perturbation theory treating discreteness as a small perturbation to the continuum. For $l_0=4$, which is the region where the perturbation starts to break down, we find that $\Delta_{\rm PN}/U_0=2(\omega_{\rm PN}/2\pi)^2/[\frac{1}{72}(\pi/l_0)^2]$ is about 3.5%. As l_0 increases the term $(\omega_{\rm PN}/2\pi)^2$ decreases much faster than U_0 so that the only correction due to discreteness is $\exp\{\beta E_K^0[\frac{1}{72}(\pi/l_0)^2]\}$ as found in Refs. 2 and 6. Thus for $l_0 \gg \pi$ we find of the two effects due to discreteness, namely, the X-independent reduction of the kink free energy U_0, and the X-dependent PN potential, only U_0 is important for large l_0 as far as statistical mechanics is concerned. At $l_0 \approx \pi$ the X-dependent potential effects are just starting to become important. In the next section we show that as l_0 becomes less than π there is a rapid growth in the magnitude of the X-dependent effects and they become larger than U_0.

V. NONPERTURBATIVE TREATMENT OF THE FREE ENERGY

In the nonperturbative region where $l_0 \le \pi$ we simplify Eq. (2.7a) for $V^{(2)}(X)$ by replacing $\hat f_i(X)$ by $f_i(\frac{1}{2})$ in all terms where a linear or quadratic term in q_i appears. Then $V_{\rm int}=0$ rigorously because f_i satisfies the exact ground-state equation,

$$f_{i+1}+f_{i-1}-2f_i-\left[\frac{\pi}{l_0}\right]^2\sin f_i=0 . \tag{5.1}$$

Equation (5.1) should be contrasted with the equation $\partial^2 f_n/\partial n^2-(\pi/l_0)^2\sin f_n=0$ which is satisfied by the function $\bar f_n(X)=4\tan^{-1}\{\exp[\pi(n-X)/l_0]\}$ that we used in Sec. IV. Since $V_{\rm int}=0$ the Hamiltonian consists of a sum, $H=H_K+H_p$. The phonon Hamiltonian is

$$H_p=\frac{1}{2}\sum_k{}' (p^2_{(k)}+\omega^2_k q^2_{(k)}) , \quad (5.2)$$

where $\omega^2(k)$ s given by Eq. (3.7). Since we have assumed that the dispersion law for $\omega(k)$ is the same in the presence as in the absence of the kink we are able to evaluate the phonon free energy even though we do not know the phonon modes of the discrete SG analytically. H_p actually contains a term $p^2_{(1)}+\omega^2_{\rm PN}q^2_{(1)}$ which comes from the bound state but the constraints in Eq. (3.8) require $p_{(1)}$ and $q_{(1)}$ to be zero. Thus we anticipate the cancellation in Eq. (3.8) due to the constraints by the prime on the sum that restricts the sum to the phonon modes. Consequently the final contribution of the phonons to the free energy is $\exp(\sigma_d)$ with σ_d given by Eq. (3.10). The P integration is given by Eq. (3.9) as before. Exact simulations show that the discrete corrections to $M(X)$ for $l_0 \le 2$ are, surprisingly, small and so we neglect the discreteness corrections to $M(X)$ for all cases. Consequently, we are left with Eq. (3.11) with $V_K(X)$ given by Eq. (2.7b).

When substituting Eq. (5.1) into Eq. (2.7d) in order to make $V_{\rm int}$ vanish, we must ask the important question of whether or not the coupling terms in $\hat{f}_i$ and q_i can be replaced by f_i and q_i. The two important physical effects contained in the correlations between $\hat{f}_i$ and q_i that are not contained in f_i and q_i are radiation of phonons and the dynamical dressing of the kink by phonons. We discuss first the radiation effect.

As l_0 decreases below π more particles become trapped in the PN well (for $l_0=2$ all nonrelativistic particles are trapped). We have found in simulations[8] that the radiation from trapped particles is weak, e.g., for $l_0=2.7$ the kink lifetime was greater than 2000 oscillations of the kink even when it started at the top of the well. For unbounded orbits that are just untrapped the radiation is larger than the trapped case but still perturbative. The energy radiated by relativistic particles is a consequence of the presence of the PN well which is the X-dependent correction to U_0. For relativistic particles with $l_0 \ge \pi$ the correction amounts to only a few percent giving rise to a shallow PN potential well. Highly relativistic particles for $l_0<\pi$ radiate nonperturbatively but in this paper we consider only nonrelativistic particles. Therefore the radiation effects not taken into account by using f_i and q_i instead of $\hat{f}_i$ and q_i are negligible for the cases we consider.

The second effect that depends on kink-phonon interactions is dynamical dressing. Since we use the exact ground state f_i and the exact shape mode there is no dynamical dressing for small oscillations. For highly nonlinear oscillations the magnitude of the dynamical dressing of $f_i(\frac{1}{2})$ is small. Furthermore we partially compensate for the neglect of the dressing in our model by using the exact $\omega_{\rm PN}$ calculated in Ref. 8 and by taking the exact value U_0 from simulation. We verify our statement about the trapping velocity by calculating the trapping velocity from the condition $\frac{1}{2}MV^2=\Delta_{\rm PN}=2M(\omega_{\rm PN}/2\pi)^2$ which gives for the trapping velocity the condition $V_{\rm trap}=\omega_{PN}/\pi$. For $l_0=2$, $V_{\rm trap}=0.333$. In our units the velocity V is dimensionless and 0.333 means a velocity of one third the speed of sound. The average thermal velocity $v_r=1(\beta M_0)^{1/2}$ is small because the dilute-kink limit requires $\beta M_0 \gg 1$.

Although we have used the property that $f_i(\frac{1}{2})$ satisfies Eq. (5.1) in order to argue that $V_{\rm int}=0$ it is important to retain the full X-dependent function $\hat{f}_i(X)$ in $V_K(X)$ so that we can include the nonlinear behavior of the kink in the PN well including trapping which plays an important role as we see below for $l_0<\pi$. Therefore we retain $\hat{f}_i(X)$ in $V_K(X)$ even though we do not have a way to justify the ansatz by an analytic expansion in a small parameter. In Sec. IV we similarly assumed the full dispersion law for a discrete chain even though our expansion in the parameter $(\pi/l_0)^2$ only justified retaining the terms up to k^4. Evaluating $V_K(X)$ in Eq. (2.7b) exactly would require a large amount of computation, however we know $V_K(X)$ is a periodic function of X so that

$$V_K(X)=U_{\rm dc}+\sum_{n=1} b_n(l_0)\cos(2\pi nX) . \quad (5.3a)$$

Further we know that b_n decreases rapidly with increasing n. Consequently we assume that we can terminate the series in Eq. (5.3a) to obtain

$$V_K(X)=E^0_K+U_0-M_0\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2+M_0\left[\frac{\omega_{\rm PN}}{2\pi}\right]^2\cos(2\pi X) \quad (5.3b)$$

and we will take U_0 from simulation, Fig. 1, and we use the exact $\omega_{\rm PN}$.[8] Since U_0 is exact and the exact $\omega_{\rm PN}$ is determined by all harmonics (with the $n>1$ terms giving relatively small corrections) we have partially compensated for the terminating of the series at $n=1$. In Eq. (5.3b) we made use of the fact that for a single harmonic, $\cos(2\pi X)$, the depth of the potential scales as the square of the PN frequency. When we substitute Eq. (5.3b) in Eq. (3.11) and use the definition of the free energy per unit volume Eq. (3.3), we obtain

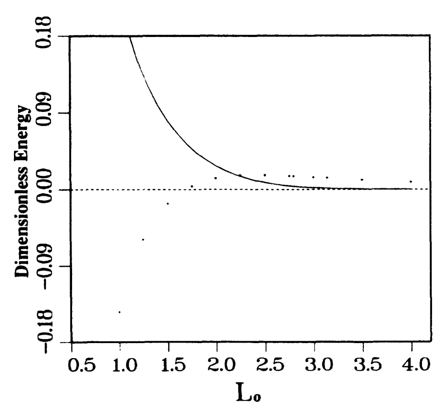

FIG. 1. The solid curve represents the quantity $(\omega_{\rm PN}/2\pi)^2$ and the dots represent the quantity $-U_0/E^0_k$. The dashed line indicates the zero of energy.

$$g-g_0=-kT\langle n_d\rangle$$
$$=-kT(2\pi\beta E_K^0)^{1/2}\frac{1}{l_0}e^{-\beta E_K^0[1-\alpha(l_0)]}$$
$$\times I_0\left[\frac{\beta\Delta_{\rm PN}}{2}\right]l^\sigma d\ , \qquad (5.4)$$

where $\alpha(l_0)\equiv-U_0/E_K^0+(\omega_{\rm PN}/2\pi)^2$ and $\Delta_{\rm PN}$ is the depth of the PN well.

VI. DISCUSSION OF RESULTS

We first compare the results of the perturbation theory of Sec. IV with the results of simulation. The details for finding $\omega_{\rm PN}$ from simulation are given in Ref. 8 and the details for finding U_0 from simulation are given in Ref. 3. For $l_0=4$, the constant $U_0/M_0=-\frac{1}{72}(\pi/l_0)^2$ is 2.9% smaller than the essentially exact simulation results. The quantity $(\omega_{\rm PN}/2\pi)^2$ (which is equal to $|C_1|/M_0$) is 4.4% larger than the simulation result, see Fig. 1. Furthermore the simulation result for the ratio of $\Delta_{\rm PN}/U_0$ is 3.2%. The argument of the modified Bessel function, $\beta E_K^0(\omega_{\rm PN}/2\pi)^2$, is $1.4\times10^{-4}\beta E_K^0$. The parameter βE_K^0 has to be greater than one to justify the dilute-kink phenomenology and a typical value would be around ten. Consequently we can replace I_0 by 1 for $l_0>3$. In summary, for $l_0\gg\pi$ the first-order perturbation theory which treats discreteness as a small perturbation has only two effects. First the phonon function σ_c is replaced by σ_d and the kink rest energy E_K^0 is reduced to $E_K^0[1-\frac{1}{72}(\pi/l_0)^2]$ making it slightly easier to create a kink which is exactly the result found in Ref. 6. Although the perturbation theory starts breaking down around $l_0\approx4$, the trend observable in perturbation theory, i.e., $\alpha(l_0)$ remaining monotonic (see Table I) regardless of the change in sign of U_0, persists in the exact simulations. For $l_0\le2.5$ the well depth $\Delta_{\rm PN}$ is actually larger than the shift of the top of the PN well, U_0, see Fig. 2. For the entire range of validity of the perturbation theory, $l_0>5$, the constant shift U_0 is negative, i.e., the PN well is depressed below the kink rest energy. For $l_0\le1.7$, U_0 is positive and thus the top of the PN well is greater than E_K^0 as shown in Fig. 2. However, the parameter $\alpha(l_0)\equiv-(U_0/E_K^0)+(\omega_{\rm PN}/2\pi)^2$ is always positive (see Table I) and is a monotonic increasing function as l_0 decreases. $\alpha(l_0)$ increases by a factor of 10 when l_0 decreases from $l_0=4$ to $l_0=1$, i.e., from 9×10^{-3} to 9×10^{-2}.

Next we show that the term $I_0[\beta E_K^0(\omega_{\rm PN}/2\pi)^2]$ can be replaced by one with a renormalized $\alpha(l_0)$ for the important region $2\le l_0\le3$, while for $l_0<2$ the full functional dependence of I_0 must be kept. The function $I_0(z)\approx1+z^2/4$ for small z and thus for small z we can express $I_0[\beta E_K^0(\omega_{\rm PN}/2\pi)^2]$ as $\exp\{[\beta E_K^0(\omega_{\rm PN}/2\pi)^2]^2/4\}$. When we substitute the preceding expression for I_0 in Eq. (5.4) we obtain

TABLE I. The parameter $\alpha(l_0)$ for various values of l_0.

l_0	$\alpha(l_0)$
1.0	0.0878
1.5	0.0641
2.0	0.0406
2.5	0.0251
3.0	0.0166
3.5	0.0119
4.0	0.0090

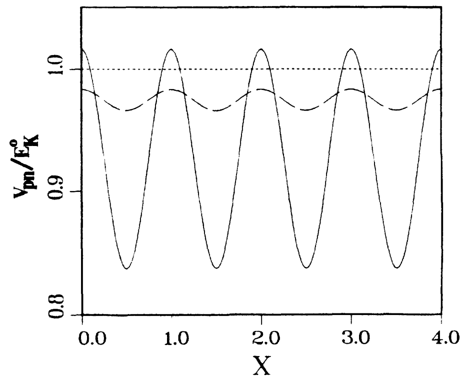

FIG. 2. The (normalized) Peierls-Nabarro potential as a function of X. The dot-dashed curve represents $l_0=2.5$ and the solid curve $l_0=1.5$. Crest and trough values are calculated using Eq. (2.4b) where we replace $\hat f_i+q_i$ by the exact kink configuration from simulation. We then fit the crest and trough values using a single cosine term to produce the figure. The dashed line represents the continuum kink rest energy $8\pi/l_0$.

$$e^{-\beta E_K^0[1-\alpha(l_0)]}I_0[\beta E_K^0(\omega_{\rm PN}/2\pi)^2]\approx e^{-\beta E_K^0[1-\bar\alpha(l_0)]}\ , \qquad (6.1)$$

where

$$\bar\alpha(l_0)\equiv-U_0/E_K^0+(\omega_{\rm PN}/2\pi)^2[1+\beta E_K^0(\omega_{\rm PN}/2\pi)^2/4]\ .$$

Thus the net effect is that I_0 can be replaced by one and the PN frequency term $(\omega_{\rm PN}/2\pi)^2$ is increased. For $l_0=2$ and $\beta E_K^0\sim10$ the term $(\omega_{\rm PN}/2\pi)^2$ is multiplied by 1.2 constituting a correction that lowers the kink rest energy. For $l_0<2$, it is necessary to retain the functional dependence of I_0.

All of the statistical thermodynamics is contained in the Helmholtz free energy and changes due to discreteness are contained in σ_d, in the constant $\alpha(l_0)$, and in the modified Bessel function $I_0(\beta\Delta_{\rm PN}/2)$. The relative lowering of the kink rest energy due to discreteness, U_0/M_0, dominates the relative effect of the PN well, $(\omega_{\rm PN}/2\pi)^2$, for most l_0, e.g., at $l_0=3$, $(\omega_{\rm PN}/2\pi)^2$ is only 17% of U_0/M_0. However, for $l_0<3$ the effect of the well increases rapidly in relative importance so that at $l_0=2$, the $(\omega_{\rm PN}/2\pi)^2$ term is more than twice as large as U_0/M_0.

In terms of the microscopic variables, X and P, for $l_0>5$ the kink behaves effectively as a free continuum particle with a reduced mass. For $3.5\le l_0\le5$ the particle sees a weak periodic PN potential which is less than 1% of the renormalized kink rest energy, with very little trapping and very weak radiation. As l_0 decreases below 3.5 the depth of the PN well, Δ_{PN}, increases and more and more particles are trapped and for $l_0 \leq 2.5$ the well depth becomes larger in magnitude than the kink energy renormalization. The radiation plays a much larger role than before but the trapped and near trapped particles radiate only a small fraction of their PN potential energy. By $l_0 \sim 2$ all particles with velocities less than one third the speed of sound are trapped and oscillate with a very small radiation rate. Kinks for which $l_0 \sim 2$ moving with velocities very near the speed of sound rapidly radiate and become trapped, radiating weakly after trapping. The phenomenon of trapping of ultrarelativistic kinks for $l_0 \leq 2$ requires large particle-phonon correlations which we explicitly excluded in our approximations in Secs. IV and V.

In conclusion, with classical mechanics discreteness constitutes a small correction to the continuum SG dilute-kink phenomenology except for kinks with $l_0 < 3$ where trapping and radiation become important. However, for non-dilute-kink problems such as kink structures on surfaces where the temperature is relatively lower and where there is a mismatch between surface and substrate one finds that pinning plays an important role at larger values of l_0 than 3. When two solitons of the continuum SG collide with each other they emerge from the collision with only a change of phase. The collision of SG kinks in a discrete lattice can cause the exchange of energy between the kinks and with the lattice undergoing such phenomena as pinning and depinning by means of collisions because in the discrete case the kink-kink interactions are taking place in the external field $V_K(X)$ of the lattice. Consequently the two particle effects which are corrections to the ideal discrete kink limit will have appreciable observable effects. The treatment of the Dirac-bracket theory of constrained Hamiltonian systems of the ideal-gas phenomenology of the nonlinear discrete SG system applies using the center of mass X in exactly the same manner in the discrete ϕ^4, DSG cases as well. Both the ϕ^4 and DSG have internal oscillations that can be represented as additional collective variables so the exchange of energy between the internal variables, the kink center of mass, and the lattice lead to interesting phenomena that have important physical applications. Quantum mechanics limits the applicability of the classical mechanics of the present paper when the uncertainty in position, ΔX, satisfies $\Delta X > a$, where a is the lattice spacing and where $\Delta X \sim \hbar(\beta/M_0)^{1/2}$ at temperature T. Consequently, at sufficiently low temperature $\Delta X \gg a$. The other temperature condition $\beta M_0 \gg 1$ is a low-temperature requirement. For a wide range of masses we are able to satisfy both the diluteness condition $\beta M_0 \gg 1$ and the condition $a \gg \hbar(\beta/M_0)^{1/2}$ required for the validity of classical mechanics in the ideal-kink-gas phenomenology of the discrete SG.

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