PHYSICAL REVIEW B VOLUME 35, NUMBER 7 1 MARCH 1987

Hamiltonian dynamics of the double sine-Gordon kink

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(Received 14 July 1986)

We present a complete Hamiltonian treatment of a kink with an internal degree of freedom, namely the double sine-Gordon (DSG) kink. In this formalism we assign two canonical coordinates and their associated momenta to describe the motion of the center of mass of the DSG kink and the relative motion of its two subkinks. We show that the canonical coordinate representing the separation of the two subkinks describes a nonlinear oscillatory degree of freedom. Consequently, the DSG kink behaves like a "molecule" (4π kink) comprised of two "atoms" (each of a single 2π kink) held together by a nonlinear potential. As an application of our formalism, we obtain the solutions for the nonlinear internal motion of the DSG in the absence of the radiation field.

I. INTRODUCTION

There has been increasing interest in the double sine-Gordon equation (DSG) because of the large number of physical phenomena which involve DSG kinks or solitons. DSG kinks have been used to model systems in condensed matter,[1–7] quantum optics,[8] and particle physics.[9] Condensed-matter applications include the spin dynamics of superfluid ^{3}He (Refs. 1 and 2), magnetic chains,[3] commensurate-incommensurate phase transitions,[4] surface structural reconstructions,[5] and domain walls.[6,7] In quantum optics and quantum field theory DSG equation applications include self-induced transparency[8] and quark confinement,[9] respectively.

The many realizable applications of the DSG model have spurred investigations into its basic structural, dynamical, thermodynamical, and critical properties.[10] Burt[11] has derived multiple soliton solutions for the DSG equations, while Iwabuchi[12] studied the commensurate-incommensurate phase transition in the DSG system. De Lillo and Sodano[13] proposed an ansatz for the analysis of the internal small-oscillation mode, subsequently, Giachetti *et al.*[14] attempted to explore its effect on the statistical mechanics of DSG kinks, while de Martino *et al.*[15] investigated the critical properties of the quantum DSG version. Condat *et al.*[16] have also explored the thermodynamical properties of the DSG chain in the different regimes of the DSG potential. Furthermore, Campbell *et al.*[17] studied, numerically, the DSG kink-antikink interactions where they demonstrated the existence of resonance exchange of energy between the translational and internal degrees of freedom of the soliton-antisoliton pair. Recently, we have extended the analysis of the small oscillations about the DSG kink beyond the ansatz level and were able to derive the complete set of eigenfunctions.[18]

In this paper we develop a complete Hamiltonian dynamics for a DSG kink where in addition to the sine-Gordon field we introduce two particle variables $X(t)$, $R(t)$ and their conjugate momenta as canonical coordinates. The variable $X(t)$ is the coordinate of the center of mass of the kink and the variable $2R(t)$ is the distance between the centers of the two subkinks that make up the DSG kink. We show that $R(t)$ describes an internal nonlinear oscillatory degree of freedom. Consequently the DSG kink behaves as if it were a "molecule" (4π kink) composed of two "atoms" (each of a single 2π kink) held together by a nonlinear potential. Since the introduction of the variables X, P_X, R, and P_R increases the number of canonical variables by four, it becomes necessary to add four constraint conditions so that the total number of independent degrees of freedom of the problem is conserved. The present work is a generalization of the approach developed by Tomboulis[19] in field theory for the single sine-Gordon kink to the case of the DSG kink. In previous papers[20,21] we demonstrated that the Tomboulis[19] approach could be generalized to the discrete sine-Gordon case. In this paper we carry out the derivation in the continuum limit; however, the analysis of the discrete case proceeds in the same manner provided that the derivatives and integrals are replaced by finite differences and sums, respectively. For convenience we treat the kink motion nonrelativistically.

The organization of this paper is as follows. In Sec. II we introduce the equations for the constraints and derive the canonical transformation to a Hamiltonian that includes the four-particle variables as canonical coordinates. We derive the equations of motion in Sec. III. In Sec. IV we discuss some significant special cases. We solve the nonlinear equation of the internal motion of the DSG kink in the absence of the radiation field in Sec. V. Section VI contains the summary and conclusions.

II. CANONICAL TRANSFORMATION AND HAMILTONIAN

We start with the Lagrangian for the discrete lattice case, anticipating future lattice applications, then we take the continuum limit for this paper. The Lagrangian for the DSG chain is

$$\bar{L}=\frac{m}{2}\sum \dot{y}_n^2-\frac{\mu}{2}\sum \left[y_{n+1}-y_n\right]^2-\frac{W}{2}\sum V\left[\frac{y_n}{a}\right], \quad (2.1)$$

where an overhead dot indicates a time derivative. a and $W/2$ are the period and amplitude of the underlying periodic potential V, respectively. μ is the force constant of the springs, m is the mass of the particle, and y_n is the displacement of the nth particle from the $2n$th trough of the underlying potential. When we introduce dimensionless variables in Eq. (2.1), we obtain

$$L\equiv(a^2\mu)^{-1}\bar{L}$$
$$=\tfrac{1}{2}\sum \dot{Q}_n^2-\tfrac{1}{2}\sum (Q_{n+1}-Q_n)^2-\frac{1}{4l_o^2}\sum V(Q_n)\ , \quad (2.2)$$

where $Q_n\equiv y_n/a$, the dimensionless time is $\tau\equiv\frac{1}{2}\omega_m t$, the square of the frequency ω_m is $\omega_m^2=4\mu/m$, l_0 is the dimensionless coupling constant which is defined as $l_0^2\equiv(\pi/2)^2(\omega_m/\omega_s)^2$, where $\omega_s^2\equiv 2\pi^2a^{-2}(W/m)$. A large value of l_0 corresponds to the case where the harmonic forces between the particles are larger than the force due to underlying periodic potential.

When we take the contiuum limit of Eq. (2.2), we obtain

$$(4\pi)^2L=\int dx\,\mathscr{L}=\int dx\left[\tfrac{1}{2}\dot{\phi}^2-\frac{1}{2}\left[\frac{\partial\phi}{\partial x}\right]^2-\left[\frac{2\pi}{l_0}\right]^2V(\phi)\right], \quad (2.3)$$

where $4\pi Q_n\leftrightarrow\phi$, $n\leftrightarrow x$, and

$$-V(\phi)\equiv 4(\cosh R)^{-2}\left[\tfrac{1}{4}\sinh^2 R(\cos\phi-1)-\left[1+\cos\frac{\phi}{2}\right]\right]. \quad (2.4)$$

The DSG potential $V(\phi)$, qualitatively, exhibits three distinct topographies depending on the parameter R. Each of these topographies has a completely different set of solutions associated with it. A complete classification of these regimes of $V(\phi)$ as a function of R and a detailed analysis of the associated solutions are given in Ref. 17 and in terms of an alternative parameter η in Ref. 13. We should point out, however, that $V(\phi)$ of Ref. 13 is not normalized as a function of η, while that of Ref. 17 is normalized such that the bottom of continuum of small oscillations about the DSG kink is always unity. We should also mention that the parameter R in Eq. (2.4) is the same as the variable R in Sec. V of Ref. 17. In the present paper we will consider only the regime defined by $R\geq 0$; the configuration of the system in this regime is shown schematically in Fig. 1(a).

We now express ϕ as the static kink solution of the DSG, which is shown in Fig. 1(b) and which we denote by σ, plus a radiation field χ such that

$$\phi(x,t)\equiv\sigma(x,X(t),R(t))+\chi(x,t)\ , \quad (2.5a)$$

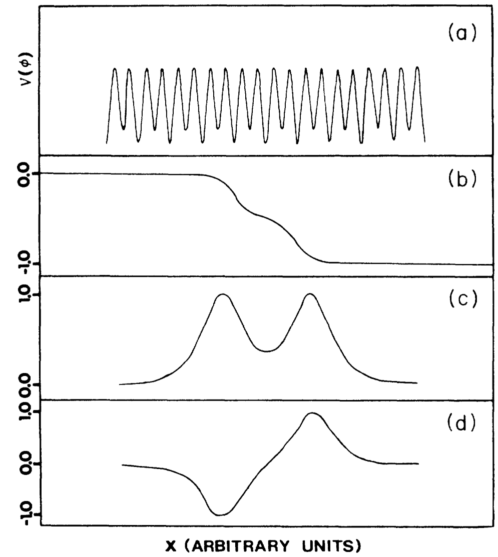

FIG. 1. (a) The double sine-Gordon potential for $\mathscr{R}\geq 1.25$, (b) solution to the DSG equation showing the two constituent subkinks separated by $2R$, (c) the small oscillations wave function $\partial\sigma/\partial X$ corresponding to the Goldstone mode, and (d) the approximate small oscillations wave function $\partial\sigma/\partial R$ corresponding to the internal degree of freedom.

where

$$\sigma(x,X,R)=\sigma_{\rm SG}\left[\frac{2\pi}{l_0}(x-X)+R\right]-\sigma_{\rm SG}\left[R-\frac{2\pi}{l_0}(x-X)\right] \quad (2.5b)$$

and

$$\sigma_{\rm SG}(x)=4\tan^{-1}[\exp(x)]\ . \quad (2.5c)$$

Equation (2.5b) expresses the interesting fact[14,17] that the static kink solution of the DSG equation can be rigorously expressed in terms of the single kink solutions of the sine-Gordon equation. The parameters X and R in Eqs. (2.5b) and (2.5c) are now to be promoted to dynamical variables $X(t)$ and $R(t)$ in order to proceed to develop a Hamiltonian formalism[19,20] in which they become canonical coordinates. The time derivative of Eq. (2.5a) is

$$\dot{\phi}=\dot{X}\frac{\partial\sigma}{\partial X}+\dot{R}\frac{\partial\sigma}{\partial R}+\dot{\chi}\ , \quad (2.6a)$$

where we use the fact that the field χ is an independent dynamical variable, i.e., it does not depend, explicitly, on $X(t)$ and $R(t)$, and we define

$$\frac{\partial\sigma}{\partial X}=\left[\frac{2\pi}{l_0}\right]\left[2\,\mathrm{sech}\left[R+\frac{2\pi}{l_0}(x-X)\right]+2\,\mathrm{sech}\left[R-\frac{2\pi}{l_0}(x-X)\right]\right], \quad (2.6b)$$

$$\frac{\partial\sigma}{\partial R}=2\,\mathrm{sech}\left[R+\frac{2\pi}{l_0}(x-X)\right]-2\,\mathrm{sech}\left[R-\frac{2\pi}{l_0}(x-X)\right], \tag{2.6c}$$

which are shown in Figs. 1(c) and 1(d), respectively.

We now substitute Eq. (2.6a) into the first term on the right-hand side of Eq. (2.3) and obtain

$$\tfrac{1}{2}\int dx\,\dot\phi^2(x)=\tfrac{1}{2}\int dx\left[\dot X\frac{\partial\sigma}{\partial X}+\dot R\frac{\partial\sigma}{\partial R}+\dot\chi\right]^2 \tag{2.7}$$

if we were to require that

$$C_2\equiv\int dx\frac{\partial\sigma}{\partial X}\dot\chi=0 \tag{2.8a}$$

and

$$C_4\equiv\int dx\frac{\partial\sigma}{\partial R}\dot\chi=0\,, \tag{2.8b}$$

then Eq. (2.7) becomes

$$\tfrac{1}{2}\int dx\,\dot\phi^2(x)=\tfrac{1}{2}\int dx\left[\left[\frac{\partial\sigma}{\partial X}\right]^2\dot X^2+\left[\frac{\partial\sigma}{\partial R}\right]^2\dot R^2+\dot\chi^2\right]. \tag{2.9}$$

As we will see below, Eqs. (2.8a) and (2.8b) are two of the four constraints needed to render the transformation from ϕ variables to the χ, R, and X variables canonical. We carry out the integrations in Eq. (2.9) and obtain

$$\tfrac{1}{2}\int\dot\phi^2(x)dx=\tfrac{1}{2}M_X\dot X^2+\tfrac{1}{2}M_R\dot R^2+\tfrac{1}{2}\int dx\,\dot\chi^2\,, \tag{2.10}$$

where

$$M_X\equiv\int dx\left[\frac{\partial\sigma}{\partial X}\right]^2=\frac{32\pi}{l_0}\left[1+\frac{2R}{\sinh(2R)}\right] \tag{2.11a}$$

and

$$M_R\equiv\int dx\left[\frac{\partial\sigma}{\partial R}\right]^2=\frac{8l_0}{\pi}\left[1-\frac{2R}{\sinh(2R)}\right]. \tag{2.11b}$$

The cross-term integral vanishes, and

$$\int dx\left[\frac{\partial\sigma}{\partial X}\right]\left[\frac{\partial\sigma}{\partial R}\right]=0\,.$$

We observe that both M_X and M_R are independent of X. (In the discrete lattice case M_X and M_R depend on X and the cross-term integral variable does not vanish.) The canonical momenta are defined as

$$\Pi=\frac{\partial\mathscr{L}}{\partial\dot\phi}=\dot\phi;\quad \pi=\frac{\partial\mathscr{L}}{\partial\dot\chi}=\dot\chi\,, \tag{2.12a}$$

$$P_X=\frac{\partial L}{\partial\dot X}=M_X\dot X;\quad P_R=\frac{\partial L}{\partial\dot R}=M_R\dot R\,. \tag{2.12b}$$

When we substitute Eqs. (2.12) in Eq. (2.6), we obtain

$$\Pi=\pi+\frac{P_X}{M_X}\frac{\partial\sigma}{\partial X}+\frac{P_R}{M_R}\frac{\partial\sigma}{\partial R} \tag{2.13}$$

and the kinetic energy can be expressed in terms of the momenta as

$$\tfrac{1}{2}\int dx\,\dot\phi^2(x)=\frac{P_X^2}{2M_X}+\frac{P_R^2}{2M_R}+\tfrac{1}{2}\int dx\,\pi^2(x). \tag{2.14}$$

The constraints required to make the transformation[19,20] from ϕ, π to $X(t)$, $R(t)$, $P_x(t)$, and $P_R(t)$ canonical are

$$C_1\equiv\int dx\frac{\partial\sigma}{\partial X}\chi(x,t)=0;\quad C_2\equiv\int dx\frac{\partial\sigma}{\partial X}\pi(x,t)=0\,, \tag{2.15a}$$

$$C_3\equiv\int dx\frac{\partial\sigma}{\partial R}\chi(x,t)=0;\quad C_4\equiv\int dx\frac{\partial\sigma}{\partial R}\pi(x,t)=0\,. \tag{2.15b}$$

We note that C_2 and C_4 are just the conditions of Eq. (2.8). The old variables satisfy the canonical Poisson bracket relations

$$\begin{aligned}&\{\phi(x),\phi(x')\}=\{\Pi(x),\Pi(x')\}=0\,,\\&\{\phi(x),\Pi(x')\}=\delta(x-x')\,.\end{aligned} \tag{2.16}$$

If we assume that the new variables satisfy $\{\chi(x),\pi(x')\}=\delta(x-x')$, we find that the Poisson brackets of the constraints lead to

$$\{C_1,C_2\}=M_X;\quad \{C_3,C_4\}=M_R\,,$$

$$\{C_1,C_3\}=\{C_1,C_4\}=\{C_2,C_3\}=\{C_2,C_4\}=0\,,$$

which violates our requirement that $C_1=C_2=C_3=C_4=0$. In Dirac's terminology[22] 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

$$\begin{aligned}\{\chi(x),\pi(x')\}&=\delta(x-x')-\{\chi(x),C_2\}[\{C_2,C_1\}]^{-1}\{C_1,\pi(x')\}-\{\chi(x),C_4\}[\{C_4,C_3\}]^{-1}\{C_3,\pi(x')\}\\&=\delta(x-x')-\{\chi(x),C_2\}M_X^{-1}\{C_1,\pi(x')\}-\{\chi(x),C_4\}M_R^{-1}\{C_3,\pi(x')\}\\&=\delta(x-x')-\frac{\partial\sigma(x)}{\partial X}M_X^{-1}\frac{\partial\sigma(x')}{\partial X}-\frac{\partial\sigma(x)}{\partial R}M_R^{-1}\frac{\partial\sigma(x')}{\partial R}\,,\end{aligned} \tag{2.17}$$

where we have set $\{X,P_X\}=\{R,P_R\}=1$, while all other Poisson brackets vanish. Furthermore, we used the relation $\phi=\sigma+\mathcal{X}$, and Eq. (2.13) to obtain the final form of the Poisson bracket relations of Eq. (2.16).

It can be easily shown that Eq. (2.17), together with $\{X,P_X\}=\{R,P_R\}=1$ and the constraints given by Eqs. (2.15) consistently satisfy the Poisson brackets of Eq. (2.16). Consequently, the transformation to the new variables $\mathcal{X}$, π, X, P_X, R, and P_R is canonical and the new dimensionless Hamiltonian is

$$\begin{aligned}H=&\frac{P_X^2}{2M_X}+\frac{P_R^2}{2M_R}+\tfrac{1}{2}\int dx\,\pi^2(x)+\tfrac{1}{2}\int dx[\mathcal{X}'(x)+\sigma'(x)]^2\\&-4\frac{2\pi}{l_0}(\cosh R)^{-2}\int dx\left\{\tfrac{1}{4}\sinh^2(R)[\cos(\sigma+\mathcal{X})-1]-\left[1+\cos\left[\frac{\sigma+\mathcal{X}}{2}\right]\right]\right\}.\end{aligned}\tag{2.18}$$

III. EQUATIONS OF MOTION

We obtain the equations of motion for our canonical variables from the Poisson bracket relation $\dot{O}=\{O,H\}$ where in general O depends on X, P_X, R, P_R, $\mathcal{X}$, and π, and does not depend explicitly on time. We use the relationships which follow from Eq. (2.17),

$$\{\pi(x),G(\mathcal{X})\}=-\frac{\partial G}{\partial\mathcal{X}(x)}+\frac{\partial\sigma(x)}{\partial X}M_X^{-1}\int dx'\frac{\partial\sigma(x')}{\partial X}\frac{\partial G}{\partial\mathcal{X}(x')}+\frac{\partial\sigma(x)}{\partial R}M_R^{-1}\int dx'\frac{\partial\sigma(x')}{\partial R}\frac{\partial G}{\partial\mathcal{X}(x')},\tag{3.1}$$

$$\{\mathcal{X}(x),G(\pi)\}=\frac{\partial G}{\partial\pi(x)}-\frac{\partial\sigma(x)}{\partial X}M_X^{-1}\int dx'\frac{\partial\sigma(x')}{\partial X}\frac{\partial G}{\partial\pi(x')}-\frac{\partial\sigma(x)}{\partial R}M_R^{-1}\int dx'\frac{\partial\sigma(x')}{\partial R}\frac{\partial G}{\partial\pi(x')}.\tag{3.2}$$

The equations of motion for $\dot{X}$, $\dot{R}$, and $\dot{\mathcal{X}}$ are

$$\dot{X}=\{X,H\}=M_X^{-1}P_X;\quad \dot{R}=\{R,H\}=M_R^{-1}P_R,\tag{3.3a}$$

$$\begin{aligned}\dot{\mathcal{X}}=\{\mathcal{X},H\}=&\pi(x)-\frac{\partial\sigma(x)}{\partial X}M_X^{-1}\int dx'\frac{\partial\sigma(x')}{\partial X}\pi(x')\\&-\frac{\partial\sigma(x)}{\partial R}M_R^{-1}\int dx'\frac{\partial\sigma(x')}{\partial R}\pi(x')=\pi(x),\end{aligned}\tag{3.3b}$$

where the second equality in Eq. (3.3b) follows from the constraint conditions $C_2=0$ and $C_4=0$.

It is necessary to consider the variable R more carefully before obtaining the equations of motion for the canonical momenta. Up to this point the same symbol R has been used for two different physical quantities which we must distinguish. First the variable R in Eq. (2.4) for the potential $V(\phi)$ is a fixed parameter that is determined by the physical system. For example in the case of the reconstruction of solid surfaces the variable R in $V(\phi)$ is determined by the effective interaction of the surface atoms with the underlying substrate. From here on we will denote this parameter by $\mathcal{R}$ so that Eq. (2.4) becomes

$$\left[\frac{2\pi}{l_0}\right]V(\phi)\leftrightarrow V_{\mathcal{R}}(\phi)=-4\left[\frac{2\pi}{l_0}\right]^2(\cosh\mathcal{R})^{-2}\left\{\tfrac{1}{4}\sinh^2(\mathcal{R})(\cos\phi-1)-\left[1+\cos\left[\frac{\phi}{2}\right]\right]\right\}.\tag{3.4}$$

The second use of R is as $R(t)$ the dynamical variable which first appears in Eq. (2.5). We retain the symbol $R(t)$ for the canonical variable. The crucial point is that in the dynamical motion of the DSG kink the distance R between the centers of the subkinks will vary with time and thus R will be a function of time, whereas the potential energy function $V(\phi)$ is given *a priori* and fixed for the particular given physical system and thus $\mathcal{R}$ is a fixed parameter. The equations of motion for the momenta are

$$\begin{aligned}\dot{\pi}=\{\pi,H\}=\ddot{\mathcal{X}}=&\frac{\partial^2\mathcal{X}}{\partial x^2}+\frac{\partial^2\sigma}{\partial x^2}-\frac{\partial V_{\mathcal{R}}(\sigma+\mathcal{X})}{\partial\mathcal{X}}\\&-\frac{1}{M_X}\frac{\partial\sigma(x)}{\partial X}\int dx'\frac{\partial\sigma(x')}{\partial X}\left[\frac{\partial^2\mathcal{X}}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathcal{R}}(x')}{\partial\mathcal{X}(x')}\right]\\&-\frac{1}{M_R}\frac{\partial\sigma(x)}{\partial R}\int dx'\frac{\partial\sigma(x')}{\partial R}\left[\frac{\partial^2\mathcal{X}}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathcal{R}}(x')}{\partial\mathcal{X}(x')}\right],\end{aligned}\tag{3.5}$$

$$\begin{aligned}\dot{P}_X=\{P_X,H\}=&+\frac{P_X^2}{2M_X^2}\frac{\partial M_X}{\partial X}+\frac{P_R^2}{2M_R^2}\frac{\partial M_R}{\partial X}+\int dx'\frac{\partial\sigma(x')}{\partial X}\left[\frac{\partial^2\mathcal{X}}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathcal{R}}(x')}{\partial\mathcal{X}(x')}\right]\\=&\int dx'\frac{\partial\sigma(x')}{\partial X}\left[\frac{\partial^2\mathcal{X}}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathcal{R}}(x')}{\partial\mathcal{X}(x')}\right],\end{aligned}\tag{3.6}$$

where the second equality in Eq. (3.6) follows from the fact that in the continuum limit M_X and M_R are independant of X. (In the discrete lattice[11] M_X and M_R do depend on X.) The equation for $\dot{P}_R$ is

$$\dot{P}_R=+\frac{P_R^2}{2M_R^2}\frac{\partial M_R}{\partial R}+\frac{P_X^2}{2M_X^2}\frac{\partial M_X}{\partial R}+\int dx'\frac{\partial\sigma(x')}{\partial R}\left[\frac{\partial^2\chi}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathscr{R}}(x')}{\partial\chi(x')}\right]. \quad (3.7)$$

When we substitute Eq. (3.3a) for the momenta into Eqs. (3.6) and (3.7), we obtain

$$\ddot{X}=\frac{1}{M_X}\int dx'\frac{\partial\sigma(x')}{\partial X}\left[\frac{\partial^2\chi}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathscr{R}}(x')}{\partial\chi(x')}\right], \quad (3.8)$$

$$\ddot{R}=-\tfrac{1}{2}\dot{R}^2\frac{\partial \ln M_R}{\partial R}-\frac{\dot{X}^2}{2M_R}\frac{\partial M_X}{\partial R}+\frac{1}{M_R}\int dx'\frac{\partial\sigma(x')}{\partial R}\left[\frac{\partial^2\chi}{\partial x'^2}+\frac{\partial^2\sigma}{\partial x'^2}-\frac{\partial V_{\mathscr{R}}(x')}{\partial\chi(x')}\right]. \quad (3.9)$$

We can write Eq. (3.5) in the form

$$\ddot{\chi}=(1-\mathscr{P}_X-\mathscr{P}_R)\left[\frac{\partial^2\chi}{\partial x^2}+\frac{\partial^2\sigma}{\partial x^2}-\frac{\partial V_{\mathscr{R}}}{\partial\chi}\right], \quad (3.10)$$

where the projection operators $\mathscr{P}_X$ and $\mathscr{P}_R$ are defined by the relations

$$\mathscr{P}_X O(x)\equiv\frac{\partial\sigma(x)}{\partial X}\frac{1}{M_X}\int dx'\frac{\partial\sigma(x')}{\partial X}O(x'), \quad (3.11a)$$

$$\mathscr{P}_R O(x)\equiv\frac{\partial\sigma(x)}{\partial R}\frac{1}{M_R}\int dx'\frac{\partial\sigma(x')}{\partial R}O(x'). \quad (3.11b)$$

We can write Eq. (3.5) in an alternate form

$$\ddot{\chi}-\left[\frac{\partial^2\chi}{\partial x^2}+\frac{\partial^2\sigma}{\partial x^2}-\frac{\partial V_R}{\partial\chi}\right]=-\frac{\partial\sigma(x)}{\partial X}\ddot{X}-\frac{\partial\sigma(x)}{\partial R}\times\left[\ddot{R}+\frac{\dot{R}^2}{2}\frac{\partial\ln M_R}{\partial R}+\frac{\dot{X}^2}{2M_R}\frac{\partial M_X}{\partial R}\right], \quad (3.12)$$

where we used the equations of motion (3.8) and (3.9). Although Eq. (3.10) [or equivalently Eq. (3.12)] is the equation of motion for χ there is still an additional transformation we can perform that will be useful later when we linearize the equation of motion for χ. The static DSG solution $\sigma(x,X,R)$ defined in Eq. (2.5b) is a solution of the equation

$$\frac{\partial^2\sigma(x,X,R)}{\partial x^2}=\frac{\partial V_R[\sigma(x,X,R)]}{\partial\sigma}, \quad (3.13)$$

where the crucial point is that the parameter R in the potential V_R is the same R that appears as the parameter R in $\sigma(x,X,R)$. When we substitute Eqs. (3.13) in Eqs. (3.10), (3.8), and (3.9), we obtain

$$\ddot{\chi}=(1-\mathscr{P}_X-\mathscr{P}_R)\left[\frac{\partial^2\chi}{\partial x^2}+\frac{\partial}{\partial\sigma}(V_R[\sigma(R)]-V_{\mathscr{R}}[\sigma(R)+\chi])\right], \quad (3.14)$$

$$\ddot{X}=\frac{1}{M_X}\int dx'\frac{\partial\sigma(x')}{\partial X}\left[\frac{\partial^2\chi(x')}{\partial x'^2}+\frac{\partial}{\partial\sigma}(V_R[\sigma(x',R)]-V_{\mathscr{R}}[\sigma(x',R)+\chi])\right], \quad (3.15)$$

$$\ddot{R}+\tfrac{1}{2}\dot{R}^2\frac{\partial\ln M_R}{\partial R}+\frac{1}{2}\frac{\dot{X}^2}{M_R}\frac{\partial M_X}{\partial R}=\frac{1}{M_R}\int dx'\frac{\partial\sigma(x')}{\partial R}\left[\frac{\partial^2\chi(x')}{\partial x'^2}+\frac{\partial}{\partial\sigma}(V_R[\sigma(x',R)]-V_{\mathscr{R}}[\sigma(x',R)+\chi])\right]. \quad (3.16)$$

Equations (3.14), (3.15), and (3.16) constitute the complete closed set of canonical equations of motion for χ, $X(t)$, and $R(t)$.

In the next two sections we consider some relevant limiting cases of the equations of motion.

IV. LINEARIZED EQUATION OF MOTION FOR $\chi(t)$

When we linearize Eq. (3.14) for χ by expanding $V_{\mathscr{R}}[\sigma(R)+\chi]$ to first order in χ we obtain

$$\ddot{\chi}=(1-\mathscr{P}_X-\mathscr{P}_R)\Lambda\chi+(1-\mathscr{P}_X-\mathscr{P}_R)S\equiv\tilde{\Lambda}\chi+\tilde{S}, \quad (4.1)$$

where $\tilde{O}\equiv(1-\mathscr{P}_X-\mathscr{P}_R)O$. The operator Λ is

$$\Lambda\equiv\frac{\partial^2}{\partial x^2}-V''_{\mathscr{R}}[\sigma(x,R)]$$

and S is defined as

$$S\equiv V'_R[\sigma(x,R)]-V'_{\mathscr{R}}[\sigma(x,R)]. \quad (4.2)$$

The prime indicates a derivative with respect to σ. Figure 2 provides two typical examples for the spatial dependence of S corresponding to $\mathscr{R}=2.4$ and $\mathscr{R}=3.2$ with $R=2.3$ and 3.1, respectively. The explicit expression for $V''_R[\sigma(x,R)]$ is

$$
\begin{aligned}
V''_{\mathscr{R}}[\sigma(x,R)] &= \left[\frac{2\pi}{l_0}\right]^2 \left[-1+\tanh^2\mathscr{R}\cos[\sigma(x,R)]-\operatorname{sech}^2\mathscr{R}\cos\left[\frac{\sigma(x,R)}{2}\right]\right] \\
&= \left[\frac{2\pi}{l_0}\right]^2 \left[-1+\tanh^2\mathscr{R}\left[\frac{2\cosh^2 R-\sinh^2\left[\frac{2\pi}{l_0}[x-X(t)]\right]}{\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}[x-X(t)]\right]}-1\right]\right. \\
&\qquad \left. -\operatorname{sech}^2\mathscr{R}\left[\frac{\cosh^2 R-\sinh^2\left[\frac{2\pi}{l_0}[x-X(t)]\right]}{\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}[x-X(t)]\right]}\right]\right] ,
\end{aligned}
\tag{4.3}
$$

where we used the expression

$$
\cos\left[\frac{\sigma(x,R)}{2}\right]=\frac{\cosh^2 R-\sinh^2\left[\frac{2\pi}{l_0}[x-X(t)]\right]}{\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}[x-X(t)]\right]} . \tag{4.4}
$$

We can obtain an explicit expression for S by substituting Eq. (4.4) into Eq. (4.2),

$$
\begin{aligned}
\left[\frac{l_0}{2\pi}\right]^2 S(x,t) &= \left[\frac{\cosh R\sinh\left[\frac{2\pi}{l_0}\right][x-X(t)]}{\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}\right][x-X(t)]}\right][-4\operatorname{sech}^2 R(t)+4\operatorname{sech}^2\mathscr{R}] \\
&\quad + \frac{4\cosh R\sinh\left[\frac{2\pi}{l_0}\right]x\left[\cosh^2 R-\sinh^2\left[\frac{2\pi}{l_0}\right]x\right]}{\left[\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}\right]x\right]^2}[\tanh^2 R(t)-\tanh^2\mathscr{R}] .
\end{aligned}
\tag{4.5}
$$

The linear operator Λ is time dependent because the operator $V''_{\mathscr{R}}\{\sigma[x,R(t),X(t)]\}$ depends on time through $R(t)$ and $X(t)$. We show below that $R(t)$ has an oscillatory time dependence and consequently so does $\Lambda(t)$. In addition, if the center of mass $X(t)$ is accelerating it will also contribute to the time dependence of $\Lambda(t)$. Consequently, we define a time-independent operator Λ_{SCH} in the following manner.

$$
\begin{aligned}
\Lambda &= \frac{\partial^2}{\partial x^2}-V''_{\mathscr{R}}[\sigma(R(t),X(t))] \\
&= \frac{\partial^2}{\partial x^2}-V''_{\mathscr{R}}[\sigma(\mathscr{R},X_0)] \\
&\quad +\{V''_{\mathscr{R}}[\sigma(\mathscr{R},X_0)]-V''_{\mathscr{R}}[\sigma(R(t),X(t))]\} \\
&\equiv -\Lambda_{\mathrm{SCH}}+\delta\Lambda(t) ,
\end{aligned}
\tag{4.6}
$$

where

$$
\Lambda_{\mathrm{SCH}}=-\frac{\partial^2}{\partial x^2}+V''_{\mathscr{R}}[\sigma(\mathscr{R},X_0)] , \tag{4.7}
$$

where Λ_{SCH} is the "Schrödinger" equation associated with the DSG equation, i.e., the linearized DSG equation about the static kink solution $\sigma(\mathscr{R},X_0)$. The operator $\delta\Lambda(t)$ is given by

$$
\delta\Lambda(t)=V''_{\mathscr{R}}[\sigma(\mathscr{R},X_0)]-V''_{\mathscr{R}}[\sigma(R(t),X(t))] \tag{4.8}
$$

and derives its time dependence from the motion of the center of mass $X(t)$ and internal oscillation $R(t)$. Analytic expressions for the eigenfunctions and eigenvalues of

$$
\frac{\partial^2\psi}{\partial t^2}+\Lambda_{\mathrm{SCH}}\psi=0 \tag{4.9}
$$

are given in Ref. 18. The spectrum of Λ_{SCH} consists of the two discrete eigenvalues corresponding to the Goldstone mode and the shape mode in addition to the continuum which starts at $\omega=2\pi/l_0$. The shape mode is

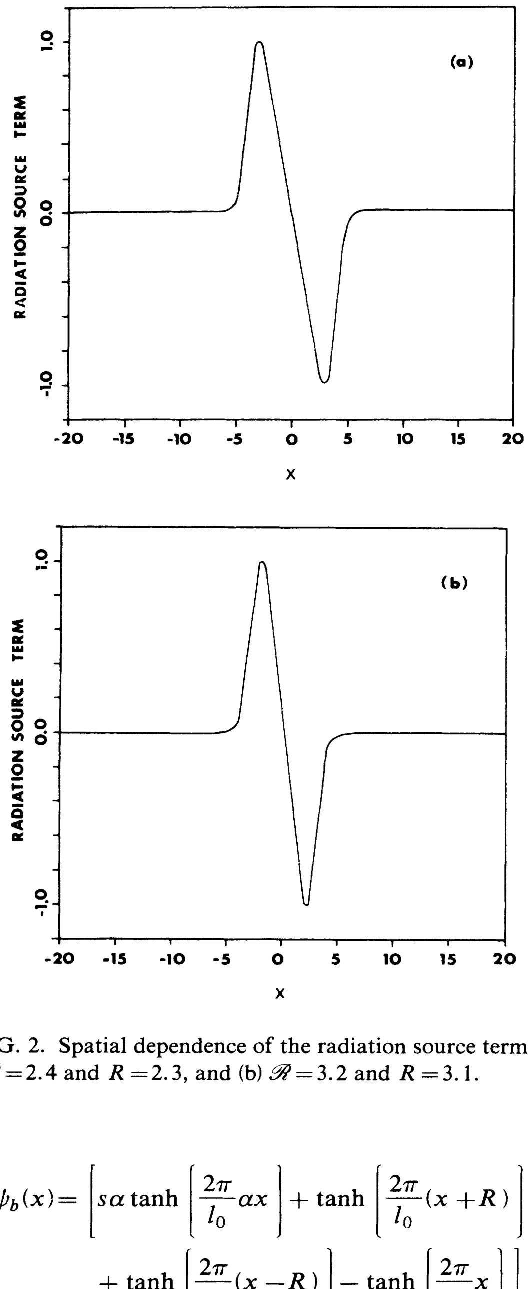

FIG. 2. Spatial dependence of the radiation source term S for (a) $\mathscr{R}=2.4$ and $R=2.3$, and (b) $\mathscr{R}=3.2$ and $R=3.1$.

$$\psi_b(x)=\left[s\alpha\tanh\left[\frac{2\pi}{l_0}\alpha x\right]+\tanh\left[\frac{2\pi}{l_0}(x+R)\right]\right.$$
$$\left.+\tanh\left[\frac{2\pi}{l_0}(x-R)\right]-\tanh\left[\frac{2\pi}{l_0}x\right]\right]$$
$$\times\left[\cosh\left[\frac{2\pi}{l_0}\alpha x\right]\right]^{-s}, \tag{4.10}$$

where

$$\alpha\equiv\tanh^2 R\frac{\sinh(2R)}{\sinh(2R)-2R},$$
$$s\equiv\tfrac{1}{2}[-1+(1+\alpha^{-2}8\tanh^2 R)^{1/2}],$$

and the eigenfrequency

$$\omega_b=\frac{2\pi}{l_0}(1-s^2)^{1/2}.$$

We refer the reader to Ref. 18 for a complete discussion of Eq. (4.9). If we consider a linear deviation from equilibrium in the original field variable $\phi=\sigma(R)+\chi$, we obtain

$$\delta\phi=\left.\frac{\partial\sigma}{\partial R}\right|_{R=\mathscr{R}}\delta R+\chi,$$

where χ satisfies Eq. (4.1). Thus we expect that

$$\psi_b(x)\sim\left.\frac{\partial\sigma}{\partial R}\right|_{R=\mathscr{R}}\delta R+\chi$$

because ψ_b is a small first-order correction about the static solution $\sigma(\mathscr{R})$. The authors of Ref. 17 observed that for $R\geq 2$ their numerically evaluated ψ_b approached $\partial\sigma/\partial R$. We find that the difference between the exact ψ_b and $\delta\sigma/\partial\mathscr{R}$ is less than 1% for $\mathscr{R}\geq 2$. Consequently, we find that the contribution to ψ_b from χ is negligible for small δR, except in the small range of $1.25\leq\mathscr{R}\leq 2.0$. However, it is possible that this contribution may become appreciable for deviations δR where nonlinear effects are important. There are two additional situations where χ will be important: First, if we have external phonons which are either high or low intensity; second, if the DSG kink radiates spontaneously, the radiated field will be described by χ. The source of spontaneous emission is $S(x,t)$ given by Eq. (4.5). We return to a discussion of spontaneous emission at the end of the next section after we have solved for $R(t)$ which is needed for a discussion of radiation.

V. SOLUTION FOR $R(t)$

In this section we shall discuss the solutions of the equation of motion for the collective variable $R(t)$ in the absence of the radiation field χ. We then obtain the corresponding solutions for $\phi(x,t)$ by substituting $R(t)$ in the function $\sigma[x,R(t)]$, i.e., for $\chi=0$ the time-dependent solution of the DSG equation is, simply, a dynamic version of the static solution with the parameter $\mathscr{R}$ replaced by the collective canonical variable $R(t)$. For ease in presentation we will go to the center-of-mass frame, which allows us to set the variable X equal to zero. When we set $\chi=0$ in Eq. (3.16), we obtain

$$\ddot{R}+\tfrac{1}{2}\dot{R}^2\frac{\partial\ln M_R}{\partial R}=\frac{1}{M_R}\int dx'\frac{\partial\sigma(x')}{\partial R}S(x')$$
$$\equiv-\frac{1}{M_R}\frac{\partial u_{\mathscr{R}}}{\partial R}, \tag{5.1}$$

where

$$v_{\mathscr{R}}(R)\equiv\int dx\left[\frac{1}{2}\left[\frac{\partial\sigma(x,R)}{\partial x}\right]^2\right.$$
$$\left.+\left[\frac{2\pi}{l_0}\right]^2 V_{\mathscr{R}}\left[\sigma(x,R)\right]\right]. \tag{5.2}$$

We observe that we could have obtained Eqs. (5.1) and (5.2) more directly by returning to Eq. (2.18) setting X, P_X, χ, and π equal to zero leaving us with a one particle

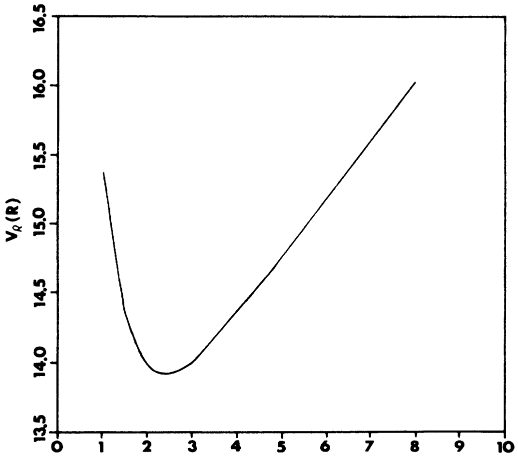

FIG. 3. The effective nonlinear potential $u_{\mathscr{R}}(R)$ for $\mathscr{R}=2.4$.

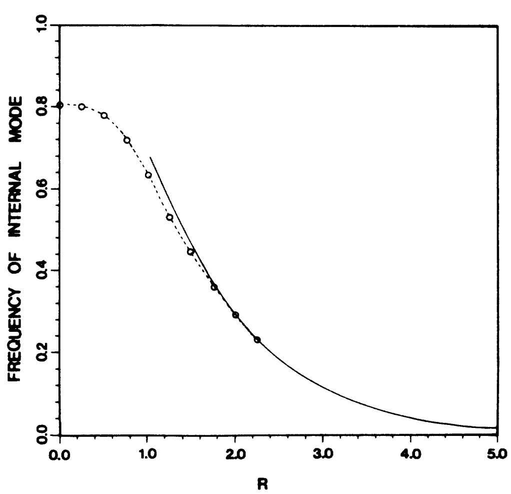

FIG. 4. Dependence of the effective internal oscillations frequency $\omega_0(\mathscr{R})$ on $\mathscr{R}$ for $\mathscr{R}\geq 1.25$ and $l_0=7.8$. The points represent the numerical calculations of Ref. 17 scaled to the bottom of the continuum at $2\pi/l_0$.

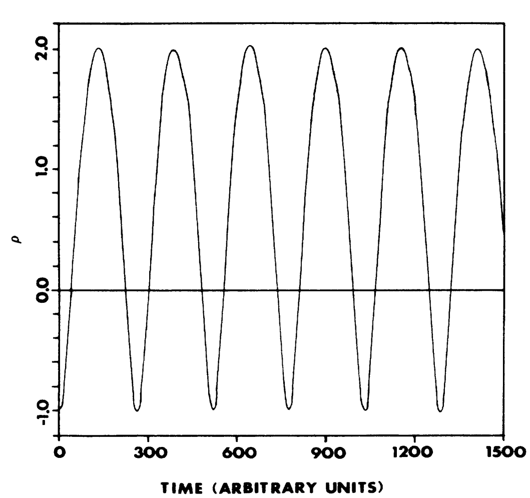

FIG. 5. The oscillatory time dependence of $\rho(t)=R(t)-\mathscr{R}$, for $\mathscr{R}=2.4$ and $\rho(0)=-1.0$.

Hamiltonian for $R(t)$. However, in that case we have to distinguish carefully between $\mathscr{R}$ and $R(t)$ so that

$$H\left[R,P_R\right]=\frac{P_R^2}{2M_R}+u_{\mathscr{R}}(R) \tag{5.3}$$

which is identical to Eq. (5.2). The result of the integrations in Eq. (5.2) is

$$u_{\mathscr{R}}(R)=8\left[\frac{2\pi}{l_0}\right]\times\left[1+\frac{\tanh^2\mathscr{R}}{\tanh^2 R}+2R\left[\frac{1}{\sinh 2R}+\frac{\coth R}{\cosh^2\mathscr{R}}-\frac{\tanh^2\mathscr{R}\cosh R}{2\sinh^2 R}\right]\right]. \tag{5.4}$$

In Fig. 3 we plot $u_{\mathscr{R}}(\rho)$ versus ρ, where $\rho\equiv R-\mathscr{R}$, for $\mathscr{R}=2.4$. We get a quantitatively different but qualitatively similar potentials for different $\mathscr{R}$'s. The single minimum of $u_{\mathscr{R}}(\rho)$ is for $\rho=0$ for all $\mathscr{R}$. Furthermore, for $\rho<0$ the potential is repulsive resisting compression of the two sub 2π kinks, while for $\rho>0$ the potential is attractive with almost a constant force. If we increase $\mathscr{R}$ the magnitude of the potential decreases and both the attractive and repulsive forces become weaker. $u_{\mathscr{R}}(\rho)$ roughly resembles the interatomic potential of a diatomic molecule. For small ρ we have harmonic oscillations about the potential minimum at $\rho=0$ with a frequency given by

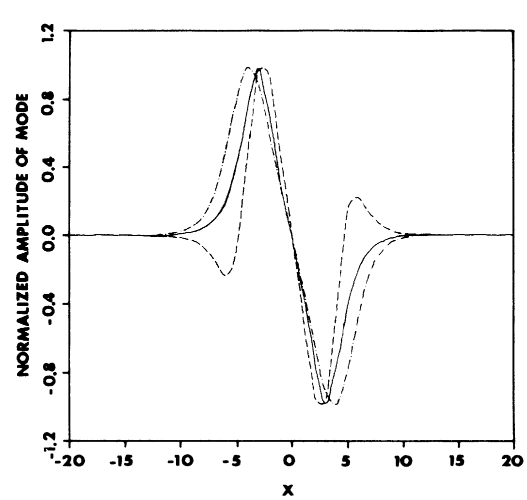

FIG. 6. The spatial dependence of the first and second harmonic parametric modes, solid and dashed lines, respectively. The shape mode is also shown for comparison, dashed-dotted curve.

$$\omega_0^2 = M_{\mathscr{R}}^{-1} \frac{\partial^2}{\partial R^2} u_{\mathscr{R}}(R) \bigg|_{R=\mathscr{R}}$$
$$= \left[\frac{2\pi}{l_0}\right] M_{\mathscr{R}}^{-1} 16 \left[\frac{1}{\sinh^2\mathscr{R}}(3-\mathscr{R}\coth\mathscr{R}) + \frac{1}{\cosh^2\mathscr{R}}(\mathscr{R}\tanh\mathscr{R}-1) - \frac{2\mathscr{R}\coth\mathscr{R}}{\cosh^2\mathscr{R}\sinh^2\mathscr{R}}\right], \tag{5.5}$$

where $M_{\mathscr{R}}$ is given by Eq. (2.11b). For large $\mathscr{R}$, $\omega_0^2(\mathscr{R})$ approaches zero as $8(2\pi/l_0)^2 e^{-2\mathscr{R}}$. While in the limit $\mathscr{R}\to 0$, $\omega_0^2(\mathscr{R})$ approaches a constant. In Fig. 4, we plot $\omega_0(\mathscr{R})$ versus $\mathscr{R}$. For $\mathscr{R} \lesssim 1.15$ the potential $V(\phi)$ has one minimum, only instead of the two minima of the DSG. Furthermore, in that range of $\mathscr{R}$, $\omega_0(\mathscr{R})$ is resonant with the continuum and the soliton will couple strongly to the phonon field. Consequently, we only present $\omega_0(\mathscr{R})$ in the range of $\mathscr{R} \geq 1.15$. In Ref. 17 the authors obtained an approximate expression for the frequency of small oscillations of the DSG kink, ω_b where

$$\omega_b^2 = \left[\frac{2\pi}{l_0}\right]^2 \left[\frac{3}{\sinh^2\mathscr{R}} - \frac{1}{\cosh^2\mathscr{R}}\left[\frac{\sinh^2(2\mathscr{R})+2\mathscr{R}}{\sinh^2(2\mathscr{R})-2\mathscr{R}}\right]\right]. \tag{5.6}$$

We find that for $\mathscr{R} \geq 1.25$ $\omega_b(\mathscr{R})$ and $\omega_0(\mathscr{R})$ differ by less than 1%.

We obtain the nonlinear solution for $\phi(x,t)=\sigma(x,R(t))$, where we have set $\chi=0$, by solving Eq. (5.1) in the center-of-mass frame where $X=0$. In Fig. 5 we show a typical solution for the $R(t)$ motion; where we plot $\rho(t)=R(t)-\mathscr{R}$ as a function of time, for $\mathscr{R}=2.4$ and $\rho(0)=-1.0$. The solution is periodic in time, but displays an asymmetry in *rho* where the positive swing is nearly double the negative one. Subsequently, we substitute the $R(t)=\mathscr{R}+\rho(t)$ solution in the expression for $\sigma(x,R(t))$ given in Eq. (2.5b), setting $X=0$. The resulting expression for ϕ describes a nonlinear internal oscillation of the DSG kink where the distance between the two subkinks, namely $2R$, follows a time evolution governed by the nonlinear potential $u_{\mathscr{R}}(R)$. We have investigated the behavior of this motion by taking the time Fourier transform of $\phi(x,R(t))$. We obtained a set of evenly spaced harmonics in the frequency spectrum. In Fig. 6 we show the spatial dependence of the lowest two harmonics; we have also plotted, on the same figure, the shape mode $\partial\sigma/\partial R$ for comparison. We notice that the first harmonic has the same general shape as $\partial\sigma/\partial R$, however, the extrema of the former appear at larger ρ values as to be expected from the large asymmetry in the ρ oscillations. We also observe that the higher harmonics have increasing number of nodes. In a future publication we will carry out a comprehensive analysis of the nonlinear oscillations including the investigation of the coupling of higher harmonics, with frequencies overlapping the radiation continuum ($\omega \geq 2\pi/l_0$), to χ, and its contribution to the damping of this motion.

VI. CONCLUSION

In this paper we have developed for what we believe to be the first time a complete, nonrelativistic Hamiltonian dynamics for a kink with an internal degree of freedom. We introduced, in addition to the sine-Gordon field, two particle variables and their conjugate momenta as canonical variables. The coupled equations of motion of the two canonical coordinates $X(t)$ and $R(t)$, as well as, those of the radiation field χ have been derived. Furthermore, a linearized version of the χ equations of motion have been obtained.

As an application of our formalism we solved the equations of motion in the absence of the radiation field χ, but with the full nonlinearity in the motion of the R coordinate. This provided us with a powerful tool to analyze the highly nonlinear internal motion of the DSG kink. However, our solution is valid only for $\mathscr{R} \geq 1.25$. For smaller $\mathscr{R}$ the effect of the radiation field is expected to be substantial, thus implying that our approximation ($\chi=0$) is invalid in this range. Our expectation is substantiated also by the linear analysis of Ref. 18 where we showed that for small $\mathscr{R}$ the normalization of the continuum eigenstates is $\mathscr{R}$ dependent; this points to the fact that in this range of the parameter the phonon modes are rigorously influenced by the presence of the kink.

Our analysis can be regarded as a canonical and fully nonlinear treatment of the motion of a wobbling kink in a model which exhibits an exact topological soliton with an internal mode. This is relevant not only for the dynamical properties of kinks in the numerous systems modeled by the DSG equation but also if extended to the study of the polaronlike solutions in polymer models could reveal interesting properties of such systems.

Finally, within the DSG model we can cite some interesting applications to our approach. One such extension of our analysis would be to inclued the effect of stochastic noise on the kink dynamics of this model. This will allow for a more detailed study of the thermodynamical properties of the DSG equation. It will also provide the tools for the investigation of a stochastic activation mechanism of the DSG kink shape mode. Another immediate application of the Hamiltonian dynamics of DSG kink is the investigation of the scattering problem of a DSG kink pair and a kink-antikink pair which has been recently studied, numerically, by Campbell *et al.*[17] We are currently working on these problems.

ACKNOWLEDGMENTS

This work is supported by the U.S. Department of Energy under Contract No. DE-FG02-85ER45222. One of the authors, P. S., would like to thank NATO for financial support.

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