PHYSICAL REVIEW B VOLUME 42, NUMBER 10 1 OCTOBER 1990

Momentum constraints in collective-variable theory

R. Boesch* and C. R. Willis
Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215
(Received 2 April 1990)

We present an analysis of the constraints used in collective-variable treatments of kink-bearing nonlinear Klein-Gordon equations, which appear in field theory and in continuum and discrete condensed-matter systems. In particular, we introduce into the collective-variable theory a family of momentum constraints that includes the momentum constraints that have been used in the literature so far. We derive the collective-variable Hamiltonian and show that there is a single member of the family of constraints for which the kinetic energy of the collective mode separates from the other variables in the theory so that a truly particle-like description of kink dynamics results. We discuss the general structure of the Hamiltonian collective-variable equations of motion and also present a simple derivation of the collective-variable theory beginning from a Lagrangian. We obtain, therefore, the correct choice of momentum constraint within the family for both Hamiltonian and Lagrangian approaches to multiple collective-variable theories.

I. INTRODUCTION

Collective-variable treatments of nonlinear Klein-Gordon equations have been successfully used for field theories[1] and for both continuum[2] and discrete[2,3] condensed-matter systems. We will hereafter denote Ref. 2 by the Roman numeral I. Various approaches such as Lagrangian dynamics with Lagrange multipliers,[3] Hamiltonian dynamics using Dirac brackets,[4] and projection-operator methods[2] have been used to derive the collective-variable equations of motion. All of the treatments have in common the introduction of constraints. All of the treatments use the same kind of constraint on the collective variable which can be thought of as determining the value of the collective variable so as to obtain the best least-squares fit to the profile in the system, see Eq. (2.6) below. However, various approaches have been used for the constraint which determines the form of the momentum conjugate to the collective variable, such as no constraint[5] on the momentum, a constraint for the momentum of the same form as the constraint on the collective variable[1,2] or a constraint for the conjugate momentum that is of a form different than the constraint[6] on the collective variable.

In this paper we introduce a family of constraints for the conjugate momentum collective variable by choosing the momentum constraint to be a function of a parameter α. As α varies we include all the constraints that have appeared in the literature. We obtain the collective-variable Hamiltonian and show that there exists a single value of α that defines the form of the collective-variable momentum such that the kinetic energy of the collective mode acquires a simple particlelike description in the Hamiltonian. The momentum constraint corresponding to that particular value of α is given by Eq. (3.7) below. For other choices of α we show explicitly that the particlelike description in the collective variable Hamiltonian is lost. In addition, we present a Lagrangian collective-variable theory using Lagrange multipliers which although known to many in the field is unpublished and is superior to a recent Lagrangian approach.[6] We will show that the momentum constraint, Eq. (3.7), used in field theory[1] and in I, is the best momentum constraint from the point of view of both Hamiltonian and Lagrangian descriptions of collective-variable theories.

In Sec. II we use the Dirac bracket in order to find the canonical transformation from the original set of variables to the set containing the collective variable. We derive the Hamiltonian and equations of motion in Sec. III and a Lagrangian approach to collective-variable theory in Sec. IV. In Sec. V we compare our results with other collective-variable theories and conclude.

II. CANONICAL TRANSFORMATION—HAMILTONIAN APPROACH

We consider a system of harmonically coupled particles of mass $m=1$ and spring constant $k=1$ subjected to a periodic substrate potential $V_s(Q_l)$. Q_l is the position of the lth particle measured with respect to the lth minimum of V_s. The only requirement on V_s is that it be such that the system supports stable kink profiles. The Lagrangian and Hamiltonian functions for the system are

$$L=\tfrac{1}{2}\sum_l \dot{Q}_l^2-V \tag{2.1a}$$

and

$$H=\tfrac{1}{2}\sum_l P_l^2+V \, , \tag{2.1b}$$

where the potential V is defined as

$$V\equiv\tfrac{1}{2}\sum_l (Q_{l+1}-Q_l)^2+\sum_l V_s(Q_l) \tag{2.2}$$

 ©1990 The American Physical Society

and represents the sum of the harmonic and substrate potentials. The momentum P_l conjugate to Q_l is

$$P_l \equiv \frac{dL}{d\dot{Q}_l} = \dot{Q}_l \ , \qquad (2.3)$$

and the equation of motion for Q_l is

$$\ddot{Q}_l + \frac{\partial V}{\partial Q_l} = 0 \ . \qquad (2.4)$$

We assume that our system admits a single-kink structure and we let the collective variable $X(t)$ denote the motion of the collective mode we wish to consider. (We consider the single-collective-variable case for simplicity and then generalize to the multiple-collective-variable case later on.) For instance, X could represent the position of the kink's center of mass, or the slope of a ϕ^4 kink[7] (representing the displacement of the ϕ^4 kink's internal mode) or the separation of subkinks in a double sine-Gordon kink.[8,9] In other words, it is important to realize that X is in general any collective mode and not necessarily a center-of-mass mode.

In order to introduce X into the system, we construct the ansatz

$$Q_l = f_l(X) + q_l \ , \qquad (2.5)$$

where $f_l(X)$ is chosen to best represent the configuration of the system and q_l is then the remaining field such that the sum of q_l and f_l satisfies Eq. (2.5). For example, one may choose $f_l(X)$ to be the kink profile of the system in the continuum limit. The q_l would then represent not only extended phonon states but quasistatic dressing of the kink function f_l. Of course, it is not necessary to choose f_l to be the continuum kink form. Any suitable choice of f_l will do. The choice of f_l will merely govern what type of approximation one would be able to make on the q_l. The function $\partial f_l/\partial X$ represents the shape of the mode corresponding to the variable X. If X is the slope of a discrete ϕ^4 kink then $\partial f_l/\partial X$ represents the approximate shape of the discretized ϕ^4 internal mode.

We now seek a canonical transformation from the old variables Q_l, P_l to the new variables q_l, p_l, X, P where p_l and P are the momenta conjugate to q_l and X, respectively. Half of the transformation is given by Eq. (2.5). What remains is to find P_l as a function of the new variables. We will see that $P_l(q_n, p_n, X, P)$ is determined up to a function $h_l(q_l, X)$ and that h_l must satisfy a differential equation [see (Eq. (2.18)]. That is, we find a family of canonical transformations to the new set of variables where a particular member of the family is chosen by specifying an appropriate h_l. We will show that nontrivial solutions for h_l exist and give one explicitly. However, we will also show that all conditions on h_l are satisfied if we choose $h_l = 0$, which merely singles out a particular member of the family of canonical transformations. The choice $h_l = 0$ was used in I for the canonical transformation.

In order to construct the canonical transformation we must first introduce two constraints to balance the two extra degrees of freedom (X and P) that have been introduced into the system. The first constraint gives meaning to the variable X by requiring the function $f_l(X)$ to be a best fit to the field Q_l in the following simple way:

$$\frac{d}{dX} \sum_l (Q_l - f_l)^2 = 0 \ . \qquad (2.6)$$

Equations (2.6) and (2.5) lead to the first constraint condition

$$C_1 \equiv \sum_l f_l' q_l \approx 0 \ , \qquad (2.7a)$$

where $\approx$ indicates Dirac's weak equality.[4] We choose the second constraint to be of the form

$$C_2 \equiv \sum_l f_l' p_l - \alpha P \approx 0 \ , \qquad (2.7b)$$

where α is real and takes on values in the range $-\infty < \alpha < \infty$. Since the collective variable X is given its meaning by Eq. (2.7a), specifying different values for α merely redefines the momenta P and p_l and does not affect the meaning of X and the q_l.

In the general case of a system with constraints the dynamical bracket that is invariant under a canonical transformation is the Dirac bracket[4] which, for two functions A and B of the new variables, is defined as

$$\{A,B\}^* = \{A,B\} - \sum_{i,j} \{A,C_i\} C_{ij}^{-1} \{C_j,B\} \ , \qquad (2.8a)$$

where the sum on i,j is over all second-class constraints,[4] the ijth element of the matrix C is given by $C_{ij} \equiv \{C_i, C_j\}$ and $C_{ij}^{-1} \equiv (C^{-1})_{ij}$. The bracket without the asterisk is the Poisson bracket defined as

$$\{A,B\}_{(q_l,p_l,X,P)} = \sum_l \left[\frac{\partial A}{\partial q_l}\frac{\partial B}{\partial p_l} - \frac{\partial B}{\partial q_l}\frac{\partial A}{\partial p_l} \right] + \frac{\partial A}{\partial X}\frac{\partial B}{\partial P} - \frac{\partial B}{\partial X}\frac{\partial A}{\partial P} \ . \qquad (2.8b)$$

Note that the Dirac bracket reduces to the Poisson bracket when there are no constraints present. Also note that for our single-collective-variable case we have that i and j each take on the values 1 and 2. Therefore, using the constraints in Eqs. (2.7a,b) and the definition of the Poisson bracket in Eq. (2.8b) we find

$$\{C_i, C_i\} = 0, \quad i = 1,2 \qquad (2.9a)$$

and

$$\{C_1, C_2\} = M(1 - \alpha b) \ , \qquad (2.9b)$$

where we have defined the kink mass M and the function b as

$$M \equiv \sum_l (f_l')^2, \quad b = \frac{1}{M} \sum_l f_l'' q_l \ . \qquad (2.9c)$$

When we calculate the matrix C^{-1} and substitute into Eq. (2.8a) we find that the Dirac bracket for our single-collective-variable case reduces to

$$\{A,B\}^*=\{A,B\}+\frac{1}{M(1-\alpha b)}(\{A,C_1\}\{C_2,B\}-\{A,C_2\}\{C_1,B\}) . \tag{2.10}$$

Note that the Dirac bracket of C_1 and C_2, i.e., $\{C_1,C_2\}^*$, is zero.

Making use of the invariance of the Dirac bracket under a canonical transformation, it is possible to determine the function $P_l(q_n,p_n,X,P)$. The same technique was also used in I. Since the Dirac bracket for the old variables is simply the Poisson bracket, we require for any functions A and B of the coordinates and momenta that the following condition holds:

$$\{A(q_l,p_l,X,P),B(q_l,p_l,X,P)\}^*=\{A(Q_l,P_l),B(Q_l,P_l)\} , \tag{2.11a}$$

where the derivatives for the bracket on the right-hand side of Eq. (2.11a) are taken with respect to the old variables Q_l and P_l. We therefore require

$$\{Q_l,Q_n\}^*=0 , \tag{2.11b}$$

$$\{Q_l,P_n\}^*=\delta_{ln} , \tag{2.11c}$$

$$\{P_l,P_n\}^*=0 , \tag{2.11d}$$

where δ_{ln} is the Kronecker delta function.

In particular if we substitute Eq. (2.5) for Q_l into Eq. (2.11b) we obtain the identity $0=0$.

Next, we substitute Eq. (2.5) into Eq. (2.11c) and obtain a differential equation of motion for P_l:

$$\delta_{ln}=(\delta_{ls}-\mathcal{P}_{ls})\frac{\partial P_n}{\partial p_s}+f_l'(1-b)\frac{\partial P_n}{\partial P}+\alpha\left[b\left[\delta_{ln}-\frac{\partial P_n}{\partial p_l}\right]+\mathcal{P}_{ls}\frac{\partial P_n}{\partial p_s}\right] , \tag{2.12}$$

where in Eq. (2.12) and from now on a sum over repeated indices is implied and

$$\mathcal{P}_{ln}\equiv\frac{f_l'f_n'}{M} \tag{2.13a}$$

is a projection operator[2] with the properties

$$\mathcal{P}_{ln}f_n'=f_l', \quad \mathcal{P}_{ls}\mathcal{P}_{sn}=\mathcal{P}_{ln} . \tag{2.13b}$$

Although Eq. (2.12) looks somewhat complicated, it is simple to solve, which we now do. First, we project Eq. (2.12) in the direction of f_l' to obtain

$$f_n'\frac{(1-\alpha b)}{M(1-b)}=\frac{\partial P_n}{\partial P}+\frac{\alpha}{M}f_s'\frac{\partial P_n}{\partial p_s} . \tag{2.14a}$$

Next, we project Eq. (2.12) in the direction $\delta_{tl}-\mathcal{P}_{tl}$ to obtain

$$(\delta_{ls}-\mathcal{P}_{ls})\left[\frac{\partial P_n}{\partial p_s}-\delta_{sn}\right]=0 . \tag{2.14b}$$

Equations (2.14b) and (2.13b) allow us to write

$$\frac{\partial P_n}{\partial p_s}=\delta_{sn}+f_s'd_n(q_r,p_r,X,P) , \tag{2.15a}$$

where d_n is an arbitrary function of the indicated variables. Then substituting Eq. (2.15a) into Eq. (2.14a) and simplifying yields

$$\frac{\partial P_n}{\partial P}=\frac{f_n'(1-\alpha)}{M(1-b)}-\alpha d_n . \tag{2.15b}$$

Integrating Eqs. (2.15a) and (2.15b) we obtain, respectively,

$$P_n=p_n+C_2d_n+g_1(q_r,X,P) , \tag{2.16a}$$

$$P_n=\frac{f_n'(1-\alpha)P}{M(1-b)}+C_2d_n+g_2(q_r,p_r,X) , \tag{2.16b}$$

where C_2 is given by Eq. (2.7b) and g_1 and g_2 are arbitrary functions of the indicated variables. Consistency between Eqs. (2.16a) and (2.16b) requires that

$$P_n=p_n+\frac{f_n'(1-\alpha)P}{M(1-b)}+C_2d_n+h_n(q_r,X) , \tag{2.17}$$

where h_l is an arbitrary function of q_l and X.

Note that taking the derivative of Eq. (2.17) with respect to P, for example, yields the right-hand side of Eq. (2.15b) with an additional term, namely $C_2\partial d_n/\partial P$, which we set to zero since it is proportional to C_2. In fact, at this point it is permissable to set the C_2 term in Eq. (2.17) to zero even *before* derivatives are taken. The reason is because C_2 is strongly equal to zero in Dirac's sense:[4] any terms appearing in the Hamiltonian that are proportional to a constraint contribute nothing to the equations of motion when the Hamiltonian is varied. Since the constraint terms that will appear in the Hamiltonian originate in Eq. (2.17) we can set C_2 equal to zero in Eq. (2.17). However, we retain the C_2 term in order to see, for completeness, if any conditions appear on the function d_n when we impose the requirement of Eq. (2.11d). Therefore, substituting Eq. (2.17) for P_n into Eq. (2.11d), performing the derivatives and simplifying, we find that terms proportional to C_2 (or equivalently d_n) cancel exactly, α drops out and that only terms proportional to h_n survive:

$$\{P_l,P_n\}^*=\frac{\partial h_l}{\partial q_n}+\frac{\partial h_l}{\partial X}\frac{f_n'}{M(1-b)}+\frac{f_l'}{M(1-b)}\frac{\partial h_n}{\partial q_r}f_r'-(l\leftrightarrow n)=0 , \tag{2.18}$$

where the symbol $(l\leftrightarrow n)$ means interchange l and n in the entire preceding expression. Thus, there are no conditions imposed on d_n, nor since it is multiplied by C_2 does d_n contribute to the equations of motion. Therefore, d_n is completely arbitrary and we set it to zero. [We note that in I the term proportional to C_2 (or equivalently d_n) in the momentum transformation, following Eq. (A15b), was set to zero but should have been retained. Consequently, the term proportional to d_n should not be present in Eq. (A29) in I. With this correction, Eq. (A29) reduces for the single-collective-variable case to Eq. (2.18) derived above, all other results of I being unaffected by the correction.]

We see that h_l must obey Eq. (2.18). One nontrivial solution to Eq. (2.18) is

$$h_l = Af_l(X) + Bq_l \ , \tag{2.19}$$

where A and B are independent arbitrary constants. The solution given by Eq. (2.19) can be verified by substitution. Since there are no conditions on A and B they are completely arbitrary and we choose $A=B=0$ and so $h_l=0$. By choosing $h_l=0$ we single out a particular member of the family of canonical transformations to the system of collective variables for a given α.

With these choices of $d_n=0$ and $h_n=0$ the particular canonical transformation we have chosen under which the Dirac brackets are invariant [subject to the constraints in Eq. (2.7)] is

$$Q_l = f_l + q_l \ , \tag{2.20a}$$

$$P_l = p_l + \frac{f_l'(1-\alpha)P}{M(1-b)} \ . \tag{2.20b}$$

We note that α dependence is in the momentum transformation and not in the coordinate transformation. For explicit examples we consider the two cases $\alpha=0$ and $\alpha=1$. For $\alpha=0$ Eq. (2.20) reduces to that of I. When $\alpha=1$, corresponding to the constraint C_2 [cf. Eq. (2.7b)] used by Igarashi and Munakata,[6] the momentum transformation becomes

$$P_l = p_l \ . \tag{2.21}$$

The momentum transformation Eq. (2.21) looks simple, but in fact it is too simple. The idea in collective-variable theory is to separate out the nonlinear collective modes from the rest of the system; but one should not separate out the collective modes in the coordinate transformation Eq. (2.5) and then neglect to do so for the momentum transformation. Eq. (2.21) makes interpretation of the Hamiltonian difficult, as we discuss in the next section.

III. COLLECTIVE-VARIABLE HAMILTONIAN AND EQUATIONS OF MOTION

In order to calculate the collective-variable Hamiltonian, we substitute the transformation Eq. (2.20) into Eq. (2.1b). Doing so and making use of Eq. (2.7b) yields

$$H = \frac{P^2}{2\overline{M}}(1-\alpha)[1+\alpha(1-2b)] + \tfrac{1}{2}\sum_l p_l^2 + V(f_l+q_l) \ , \tag{3.1a}$$

where

$$\overline{M} \equiv M(1-b)^2 \tag{3.1b}$$

is the renormalized mass. It is tempting to renormalize the mass further by defining

$$\overline{M}_\alpha \equiv \overline{M}\frac{1}{(1-\alpha)[1+\alpha(1-2b)]} \ , \tag{3.2a}$$

so that the Hamiltonian may be written

$$H = \frac{P^2}{2\overline{M}_\alpha} + \tfrac{1}{2}\sum_l p_l^2 + V(f_l+q_l) \ . \tag{3.2b}$$

The first term in Eq. (3.2b) seems to be the kinetic energy of the collective mode—but in general it is not. It is only the kinetic energy of the collective mode for the single value $\alpha=0$.

In order to show this explicitly, we consider the Hamiltonian equation of motion for $\dot{X}$ which we calculate from Eq. (3.1a) or (3.2b) using the Dirac bracket

$$\dot{X} = \{X, H\}^* \ , \tag{3.3}$$

which yields

$$\dot{X} = \frac{P}{\overline{M}(1-\alpha b)}\{(1-\alpha)[1+\alpha(1-2b)] + \alpha^2(1-b)^2\} \ . \tag{3.4a}$$

From Eq. (3.4a) we obtain

$$\frac{P^2}{2\overline{M}_\alpha} = \tfrac{1}{2}\overline{M}_\alpha \dot{X}^2 g(\alpha) \ , \tag{3.4b}$$

where

$$g(\alpha) = \left[\frac{(1-\alpha b)(1-\alpha)[1+\alpha(1-2b)]}{(1-\alpha)[1+\alpha(1-2b)]+\alpha^2(1-b)^2}\right]^2 \ . \tag{3.4c}$$

Equation (3.4b) indicates that in general $P^2/2\overline{M}_\alpha$ does not equal $\overline{M}_\alpha\dot{X}^2/2$ and therefore cannot be the kinetic energy of the collective mode. It also does no good to define $\dot{X}_\alpha^2 \equiv g(\alpha)\dot{X}^2$ in an attempt to obtain the particle-like expression

$$P^2/2\overline{M}_\alpha = \overline{M}_\alpha \dot{X}_\alpha^2/2 \ ,$$

because then $\dot{X}_\alpha$ would imply a redefinition of the velocity of the collective mode which in turn would imply a different constraint C_1 for the definition of the collective coordinate. Therefore, we note simply that Eq. (3.4b) indicates in general that the momentum of the collective mode is accounted for partially by P and partially by the other momenta p_l.

However, only for the choice $\alpha=0$ (because b is a function of time) does $g(\alpha)$ become unity yielding the particlelike description

$$\frac{P^2}{2\overline{M}_0} = \tfrac{1}{2}\overline{M}_0\dot{X}^2 \ . \tag{3.5a}$$

The Hamiltonian for the case $\alpha=0$ becomes

$$H_{\alpha=0} = \frac{P^2}{2\overline{M}} + \tfrac{1}{2}\sum_l p_l^2 + V(f_l+q_l) \ , \tag{3.5b}$$

where we used $\overline{M}_0=\overline{M}$. Equation (3.5a) shows that the kinetic energy of the collective mode is identified as the first term in Eq. (3.5b) whereas the second term in Eq. (3.5b) is the kinetic energy of the new field variables.

We contrast the $\alpha=0$ case with the case $\alpha=1$ for which the Hamiltonian takes on a completely different form:[6]

$$H_{\alpha=1}=\frac{1}{2}\sum_l p_l^2+V(f_l+q_l) \ . \tag{3.6}$$

The term one would like to associate with the kinetic energy of the collective mode has vanished in Eq. (3.6), a consequence of the inappropriately transformed momenta in Eq. (2.21). Although the kinetic energy of the collective mode, however, *is* accounted for in Eq. (3.6), it is not identifiable because it is absorbed into one term with the field kinetic energy. It therefore makes no sense to pursue the Hamiltonian theory for any value of α other than $\alpha=0$ for which the constraint C_2 defined by Eq. (2.7b) becomes

$$C_2(\alpha=0)=\sum_l f_l' p_l \approx 0 \ . \tag{3.7}$$

For completeness, however, we briefly focus on some general properties of the equations of motion derived from Eq. (3.1a), one of which (the $\dot{X}$ equation) is given by Eq. (3.4a) and other three ($\dot{q}_l$, $\dot{p}_l$, and $\dot{P}$) of which we do not include for brevity.

One obvious feature is that the first-order equations of motion are functions of α. Therefore equations of motion for the same variable corresponding to two different values of α cannot be the same. It is easy to understand why this is so: it is the constraint $C_2(\alpha)$ that gives meaning to p_l and P. Therefore, the momentum variables p_l and P have, respectively, different meanings for different values of α and must therefore be determined by a different set of equations in order that the same physics emerge.

The only variables that have the same meaning for different α are the collective *coordinates* X and the q_l since the constraint C_1 that gives meaning to these variables is independent of α. Therefore, eliminating the momenta variables from the general equations of motion derived from Eq. (3.1a), we obtain second-order (in time) equations of motion for X and the q_l that are independent of α:

$$(\delta_{ln}-\mathcal{P}_{ln})\left[\ddot{Q}_n+\frac{dV(Q_s)}{dQ_n}\right]=0 \ , \tag{3.8a}$$

$$\mathcal{P}_{ln}\left[\ddot{Q}_n+\frac{dV(Q_s)}{dQ_n}\right]=0 \ , \tag{3.8b}$$

where Eq. (2.5) for Q_l is to be substituted into Eq. (3.8) and the projection operator $\mathcal{P}_{ln}$ is defined in Eq. (2.13a). Eqs. (3.8) are the projection-operator equations that were derived in I, which treats only the $\alpha=0$ case. The form of Eq. (3.8) suggests the existence of a powerful shortcut[2] for deriving the collective-variable equations of motion. One needs only to substitute the ansatz Q_l Eq. (2.5) into Eq. (2.4) and operate with $\mathcal{P}_{ln}$ as indicated in Eq. (3.8).

In addition, when the above analysis is carried out for multiple-collective-variable systems, the same result holds rigorously: the first-order equations of motion derived using the Dirac bracket method are α dependent because the definition of the momentum variables are α dependent. The second-order equations of motion for the coordinates are independent of α and yield the projection-operator equations derived in I. The reason the results also hold true for the multiple-collective-variable case is because the mathematical structure of the multiple-variable theory[2] is the same as that of the single-variable theory, most terms in the multiple-variable theory becoming matrix counterparts of those in the single-variable theory.

In this section we have derived the collective-variable Hamiltonian as a function of α and showed that only the value $\alpha=0$ corresponds to a Hamiltonian for which the kinetic energy of the collective mode separates completely from the momenta p_l yielding a sensible particlelike description of the collective mode in the Hamiltonian. We also showed that the second-order equations of motion obtained by eliminating the momenta are α independent and yield the projection-operator equations in Eq. (3.8).

In the next section, we carry out a simple Lagrangian approach to the problem of the canonical transformation.

IV. CANONICAL TRANSFORMATION—LAGRANGIAN APPROACH

Recently, Igarashi and Munakata[6] proposed a Lagrangian approach to collective-variable theory for the case $\alpha=1$, which led them to the Hamiltonian Eq. (3.6) in which the collective mode kinetic energy does not explicitly appear. We now present a simple Lagrangian formalism[10] for the $\alpha=0$ case in order to construct the canonical transformation to the new variables that leads instead to the correct Hamiltonian Eq. (3.5b). We therefore use the constraints defined in Eq. (2.7) with $\alpha=0$:

$$C_1=\sum_l f_l' q_l \ , \tag{4.1a}$$

$$C_2=\sum_l f_l' p_l \ . \tag{4.1b}$$

We express the Lagrangian in terms of the collective variables by substituting the ansatz Eq. (2.5) into Eq. (2.1a) and adding a Lagrange multiplier λ times $\dot{C}_1$, the time derivative of the constraint C_1, to obtain

$$L=\frac{1}{2}\sum_l (f_l'\dot{X}+\dot{q}_l)^2-\sum_l V_l(f_l+q_l) -\lambda\sum_l (f_l''\dot{X}q_l+f_l'\dot{q}_l) \ , \tag{4.2a}$$

where

$$\dot{C}_1=\sum_l (f_l''\dot{X}q_l+f_l'\dot{q}_l)=0 \ . \tag{4.2b}$$

Our motivation for incorporating the time derivative of the constraint, i.e., $\dot{C}_1=0$, into the Lagrangian instead of $C_1=0$ is the following. We note that the collective-variable equations of motion that are derived from the collective-variable Hamiltonian have the property that they satisfy the equations $\dot{C}_1=0$ and $\dot{C}_2=0$. That the constraints C_1 and C_2 are zero must be supplied as an initial condition. Therefore, using $\dot{C}_1=0$ as the constraint for the Lagrangian is consistent with the properties of the equations of motion we seek and sacrifices no information. Igarashi and Munakata[6] use instead $C_1=0$ times a Lagrange multiplier. Since they do not have velocities in their constraint term, the calculation of the collective-variable Hamiltonian is quite involved. Using $\dot{C}_1=0$ instead leads to a direct dependence of the conjugate momenta on λ, which allows us to find the canonical transformation very simply and ultimately yields the more sensible collective-variable Hamiltonian Eq. (3.5b). C_2 is not incorporated into the Lagrangian since it is a function of the momenta p_l. C_2 will be incorporated differently in order to determine λ.

The momentum p_l conjugate to q_l is

$$p_l \equiv \frac{\partial L}{\partial \dot{q}_l} = f_l' \dot{X} + \dot{q}_l - \lambda f_l' \ . \tag{4.3}$$

We see that the effects of the constraint $\dot{C}_1=0$ enter into the momentum variables through the Lagrange multiplier λ. Next, we invoke the constraint C_2 in Eq. (4.1b) in order to solve for λ. We multiply Eq. (4.3) by f_l' and sum over l to obtain (invoking the summation convention)

$$0 = M\dot{X} + f_l' \dot{q}_l - \lambda M \ , \tag{4.4a}$$

where M is the kink mass given by Eq. (2.9c). Solving Eq. (4.4a) for λ we obtain

$$\lambda = \dot{X} + \frac{1}{M} f_l' \dot{q}_l \ . \tag{4.4b}$$

Then substituting Eq. (4.4b) into Eq. (4.3) we obtain

$$p_l = \dot{q}_l - f_l' \frac{1}{M} f_n' \dot{q}_n = (\delta_{ln} - \mathcal{P}_{ln}) \dot{q}_n \ , \tag{4.5}$$

where δ_{ln} is the Kronecker delta function and $\mathcal{P}_{ln}$ is the projection operator defined in Eq. (2.13).

Next, we calculate P, the momentum conjugate to X, and obtain

$$P \equiv \frac{\partial L}{\partial \dot{X}} = f_l'(f_l' \dot{X} + \dot{q}_l) - \lambda f_l'' q_l \tag{4.6a}$$

into which we insert Eqs. (4.4b) and (2.9c) to obtain

$$P = M\dot{X} + (f_l' \dot{q}_l - \dot{X} f_l'' q_l) - \frac{1}{M} f_l' \dot{q}_l f_n'' q_n \ . \tag{4.6b}$$

We simplify Eq. (4.6b) by first writing $\dot{C}_1=0$ as

$$f_l' \dot{q}_l = -\dot{X} f_l'' q_l \tag{4.7}$$

and then use Eq. (4.7) to eliminate the sums $f_l' \dot{q}_l$ that appear in Eq. (4.6b). We thus obtain for the momentum P

$$P = M(1-b)^2 \dot{X} = \overline{M} \dot{X} \ , \tag{4.8}$$

where b is defined by Eq. (2.9c) and $\overline{M}$ by Eq. (3.1b).

In order to find the momentum transformation

$$P_l = \dot{Q}_l = \dot{X} f_l' + \dot{q}_l \ , \tag{4.9}$$

we must solve for the velocities $\dot{X}$ and $\dot{q}_l$ as functions of the new coordinates and momenta. Equation (4.8) yields immediately

$$\dot{X} = \frac{P}{M(1-b)^2} \ . \tag{4.10}$$

In order to solve for $\dot{q}_l$ we substitute into Eq. (4.3) the expressions for λ [Eq. (4.4b)], $\dot{X}$ [Eq. (4.10)], make use of Eq. (4.7), and solve the resulting equation for $\dot{q}_l$ to obtain

$$\dot{q}_l = p_l - \frac{f_l' P b}{M(1-b)^2} \ . \tag{4.11}$$

Then substituting Eqs. (4.10) and (4.11) into Eq. (4.9) we obtain for the momentum transformation

$$P_l = \frac{f_l' P}{M(1-b)} + p_l \ . \tag{4.12}$$

The canonical transformation is now complete and the Hamiltonian is calculated by substituting the momentum transformation of Eq. (4.12) into the original Hamiltonian Eq. (2.1b). We obtain

$$H = \frac{P^2}{2\overline{M}} + \frac{1}{2} \sum_l p_l^2 + C_2 \frac{P(1-b)}{\overline{M}} + V(f_l + q_l) \ . \tag{4.13}$$

The term proportional to C_2 may of course be set to zero (C_2 is strongly equal to zero as discussed in Sec. II).

The Hamiltonian Eq. (4.13) corresponds to Eq. (3.1a) with $\alpha=0$. We also note that the momentum transformation Eq. (4.12) corresponds to Eq. (2.17) for the case $\alpha=0$ and $h_l=0$. Therefore, the canonical transformation derived using the Lagrangian approach above is not the most general transformation possible. The most general transformation possible consists of a further contact transformation among the coordinates as indicated by the presence of the function $h_l(q_n, X)$, in Sec. II. The function h_l appears in the derivation given in Sec. II as an "integration constant" of the differential equations arising from the utilization of Dirac brackets. In the Lagrangian approach, there is no differential equation of that nature and so the function h_l does not appear and is effectively zero. It is possible to find other canonical transformations using the Lagrangian approach (equivalent to using different functions h_l) by modifying the Lagrangian so that one again obtains the second-order equations of motion derived in I, but we have not carried out the calculation.

V. DISCUSSION AND CONCLUSION

We first comment on the work of Tomboulis, who has introduced a collective variable X into continuum nonlinear field theory by using the Dirac bracket approach to handle the constraints. For Tomboulis X represents the center of mass of the kink. His constraints are of the same form as Eqs. (4.1) of the present paper where he used continuum fields χ and π (corresponding to our discrete q_l and p_l) which are in addition functions of X. For Tomboulis the variable P then is the total momentum of the system for which $\dot{P}=0$. However, he obtains for the kinetic energy of the kink not $P^2/2\overline{M}$ but instead the more reasonable expression $P_K^2/2\overline{M}$ where $P_K=\overline{M}\dot{X}$ is the kink momentum, thus obtaining a particlelike description of the collective mode at the Hamiltonian level. Applying the above α-dependent theory with the necessary modifications for the case where the new field variables are functions of X (like Tomboulis' χ and π), we see again that only for the case $\alpha=0$ does the kinetic energy of the collective mode separate from the rest of the Hamiltonian and that Tomboulis' approach corresponds to $\alpha=0$. We further note that since Tomboulis used a Lagrangian approach in order to find the momentum transformation to the new variables, his analysis corresponds to the case $h_l=0$ (see last paragraph of the preceding section).

Igarashi and Munakata[6] have derived a collective-variable theory corresponding exactly to the case $\alpha=1$ in the present paper. Equation (3.6) is identical to their Hamiltonian [which is Eq. (16) of Ref. 6] with their *particle* mass M set equal to unity. We see they have effectively separated out the collective mode in the coordinate transformation equivalent to Eq. (2.5) but have not done so for the momentum transformation that is given by Eq. (2.21); and so the explicit kinetic-energy term of the collective mode does not appear in their Hamiltonian. The α-dependent equations of motion derived from Eq. (3.1a) using the Dirac bracket reduce for $\alpha=1$ to their equations of motion from which they did not eliminate the momenta. By the theory of Sec. III we see that the elimination of the momenta from their equations of motion yields the projection-operator equations in Eq. (3.8). Nevertheless, their Hamiltonian cannot be remedied without changing their constraint C_2 so that is corresponds to the $\alpha=0$ case.

We now address some points on collective-variable theory that Igarashi and Munakata have raised.[6] They remark that the proof of the projection method in I, which uses the Dirac bracket technique to find the canonical transformation to the system of collective coordinates (as in Sec. II above), is incomplete because the function h_l cannot be determined within the formalism and that we have therefore set h_l equal to zero "without any rational reason." Their statement is incorrect because as explained in I *any* function h_l satisfying Eq. (2.18) defines a rigorous canonical transformation to the system of coordinates containing the collective variables and there only remains the matter of choosing the particular member of the h_l family with which to work. We chose to use the transformation corresponding to $h_l=0$ since it led to the simplest canonical transformation. In fact, since Igarashi and Munakata have used a Lagrangian approach to collective-variable theory they have (see last paragraph of Sec. IV above) formulated their analysis for exactly the $h_l=0$ case. We next recall that the first-order equations of motion derived from the Hamiltonian Eq. (3.1a) are α dependent, see Sec. III. Therefore, the statement made by Igarashi and Munakata that their first-order equations of motion are "completely equivalent" to the first-order equations of motion in I is now clearly seen to be incorrect simply because their momenta ($\alpha=1$) are defined differently than in I ($\alpha=0$). Lastly, we note that Igarashi and Munakata use their theory to calculate the function $X(t)$ corresponding to the center-of-mass motion of a discrete sine-Gordon kink trapped in the Peierls-Nabarro well, compare their results with $X(t)$ calculated from the theory of Ref. 3, and they obtain disagreement. This is not surprising, however, because it was already explained in I that the theory of Ref. 3 contained an error—hence the disagreement. They do not calculate the Peierls-Nabarro frequency or radiation effects on the kink dynamics. See Refs. 11 and 12 for a detailed analysis of discreteness effects on kink dynamics in the sine-Gordon system.

In this paper we have shown that the second-order equations of motion for the coordinates Eq. (3.8) are independent of α, but that the Hamiltonian Eq. (3.1a) and its corresponding first-order equations of motion are α dependent because the meaning of the momenta P and p_l are α dependent. We have also shown that in order to correctly define the collective momentum P and obtain the proper particlelike description of the collective mode in the Hamiltonian, it is necessary to choose $\alpha=0$ corresponding to the constraint C_2 defined by Eq. (3.7).

*Present address: Laboratoire d'Optique du Réseau, Faculté des Sciences, 6 Blvd. Gabriel, 21000 Dijon, France.

[1]E. Tomboulis, Phys. Rev. D **12**, 1678 (1975).

[2]R. Boesch, P. Stancioff, and C. R. Willis, Phys. Rev. B **38**, 6713 (1988).

[3]C. R. Willis, M. El-Batanouny, and P. Stancioff, Phys. Rev. B **33**, 1904 (1986).

[4]P. A. M. Dirac, *Lectures on Quantum Mechanics* (Academic, New York, 1964).

[5]A. Combs and S. Yip, Phys. Rev. B **28**, 6873 (1983).

[6]A. Igarashi and T. Munakata, J. Phys. Soc. Jpn. **58**, 4025 (1989).

[7]D. Campbell, J. F. Schonfeld, and C. A. Wingate, Physica D **9**, 1 (1983).

[8]R. Ravelo, M. El-Batanouny, C. R. Willis, and P. Sodano, Phys. Rev. B **38**, 4817 (1988).

[9]D. Campbell, M. Peyrard, and P. Sodano, Physica D **19**, 165 (1986).

[10]R. Jackiw (private communication).

[11]R. Boesch and C. R. Willis, Phys. Rev. B **39**, 361 (1989).

[12]R. Boesch, C. R. Willis, and M. El-Batanouny, Phys. Rev. B **40**, 2284 (1989).