Nonlinear internal-mode influence on the statistical mechanics of a dilute gas of kinks: The double-sine-Gordon model

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We investigate the classical statistical mechanics of a dilute gas of double-sine-Gordon (DSG) kinks. A novel feature of our analysis is that it includes the thermodynamical effects of the nonlinear anharmonic internal motion of the DSG kink. We compute the quantitative difference in the free energy caused by the nonlinear motion of the dynamical variable R, associated with the kink's internal motion, and compare our results with those obtained in the harmonic approximation. We show that the nonlinearity in R causes the free energy to be well behaved even when the equilibrium separation of the subkinks of a DSG kink is large. We provide an exact analytical determination of the phase shift of the phonons in the presence of a DSG kink.

I. INTRODUCTION

In the last decade there has been a remarkable surge of interest in quasi-one-dimensional condensed-matter systems bearing soliton excitations.[1] Many investigations addressed the problem of evaluating the contribution of solitonic excitations to the partition function (and related thermodynamic quantities) for systems which are approximated by continuum fields. In their pioneering work Krumhansl and Schrieffer[2] (KS) investigated the classical statistical mechanics of a one-dimensional ϕ^4 chain. Their suggestion, based on intuitive arguments and confirmed to a good approximation with the transfer-integral method,[3] was that the solitons of this theory form elementary excitations which contribute to the free energy as if they were molecules of an ideal gas. This is in addition to the usual phonon contribution.

Subsequently the concepts and methods of KS were extended and improved upon by many authors.[4] It was found that in all models solitons and phonons shared free energy and internal energy. It was shown[5] that the phase-space sharing among linear (phonons) and nonlinear (kinks) objects was due to phase-shift interactions between kinks and phonons, at least when the density of kinks is low. This discovery put the ideal-gas phenomenology on a more solid basis and led to a more accurate analysis of the classical partition function for many soliton-bearing systems.[1,4] These ideas were further extended to consistently include[6] the effects of breathers in the ideal-gas phenomenology.

Among the soliton-bearing models used to describe nonlinear phenomena in real quasi-one-dimensional systems, one of the most frequently occurring is the double-sine-Gordon (DSG) system.[7] It is a Hamiltonian field theory described by

$$H=\int dx\left[\frac{1}{2}\left[\frac{\partial\phi}{\partial t}\right]^2+\frac{1}{2}\left[\frac{\partial\phi}{\partial x}\right]^2+\left[\frac{2\pi}{l_0}\right]^2V(\phi)\right] \quad (1.1)$$

with the potential $V(\phi)$ given by

$$V(\phi)=\frac{4}{1+4\eta}\left[\left[1+\cos\frac{\phi}{2}\right]-\eta(\cos\phi-1)\right]. \quad (1.2)$$

As η is varied over the range $-\infty<\eta<\infty$, this potential exhibits a variety of topologies described in detail in Ref. 8. Here we only recall that for $\eta<\frac{1}{4}$, the potential admits two different types of kinks,[8,9] while for $\eta>\frac{1}{4}$ there is only one kink—a composite-kink structure.[8,10,11] For $|\eta|\leq\frac{1}{4}$ the potential is structurally similar to the pure sine-Gordon (SG) potential.

The physical realization of the DSG theory for some condensed-matter systems prompted earlier investigations[9,12] of the thermodynamical properties of this model within the conventional scheme of the ideal-gas phenomenology. In fact, for $\eta<0$, the DSG theory provided an ideal laboratory to investigate the thermodynamics of a one-dimensional polykink system. For $\eta>0$, the contribution to the classical partition function of the internal degree of freedom[8,10,11] of the composite DSG kink was explicitly evaluated; in these computations it was assumed that the composite DSG kink behaved as a molecule with a harmonic-oscillator-like internal degree of freedom.

In this paper we revisit the problem of constructing the classical partition function of the DSG model for $\eta\equiv(sh^2R/4)>0$. In this range of η, the DSG model arises in the study of antiferromagnetic Heisenberg chains, both with Ising-like anisotropies[13] or Dzyaloshinski-Moriya antisymmetric interactions,[14] as well as in the study of $(CH_3)_4MnCl_3$ (called TMMC in the literature).[15] Recently, it has been argued[16] that, in systems of weakly coupled magnetic sine-Gordon chains modeled by an effective one-dimensional DSG theory, there is a phase transition driven by a pairing of kinks below some critical temperature T_c. This fact, as well as the potential applications of the DSG theory in the rapidly growing area of commensurate-incommensurate phase transitions,[17] and misfit surface structures [as has been demonstrated recently for the reconstructed Au(111) surface[18]] motivates a study of the thermodynamical properties of this model which includes the effects of the nonlinear anharmonic internal motion of the DSG composite kink. As we shall see, those effects modify sensibly the free energy.

Our approach uses the path-integral formalism of Ref. 19, suitably generalized to include the effect of the constraints appearing in the canonical treatment of the DSG composite kink. A key ingredient of our investigation is provided by the Hamiltonian analysis of Refs. 11(a) and 11(b), where we introduced, in addition to the translational coordinate X a new coordinate R and its canonically conjugate momentum to describe the internal motion of the DSG kink. There we showed how to account for the dynamical effects of nonlinear oscillations of the internal motion of the kink. Although these oscillations have to be sufficiently large in order to produce observable effects, their energy is still much less than the kink's creation energy thus the effect is consistently contained in the dilute DSG gas approximation. Furthermore, our explicit solution[20] of the small-oscillation equation about the DSG kink allows us to compute exactly the phase shifts of the soliton-phonon interaction; this leads to the exact density of continuum states in the soliton sector.

Our goal in the following is to evaluate the grand-canonical partition function Ξ, including the contributions from the nonlinear motion of the internal variable R. Neglecting soliton-antisoliton interactions (dilute-gas approximation), simplifies this task considerably. In fact, in this case Ξ is simply written as[5]

$$\Xi = Z_0 \exp(2e^{\beta\mu}\mathcal{Z}_1) \; , \tag{1.3}$$

where Z_0 is the partition function of the phonons in the vacuum sector, μ is the chemical potential, $\beta \equiv (1/kT)$, and $\mathcal{Z}_1 = (Z_1/Z_0)$; Z_1 is the partition function in the single-soliton sector. Thus, from (1.3), only Z_1 needs to be computed. This we shall do in the following, where the approximation invoked in our computations shall be explicitly stated.

Our analysis does not include the contribution of breathers. Inclusion of this effect is particularly difficult in the DSG theory since the analytical solution for these excitations is not yet available. Evidence for their existence has appeared, however, in the analysis of the kink-antikink scattering performed in Ref. 8. The paper is divided as follows. In Sec. II we recall the Hamiltonian theory of the DSG kink. The computation of Z_1 is done in Sec. III. In Sec. IV we compute the free energy of the dilute gas of DSG kinks. Section V is dedicated to the comparison of our result with the harmonic approximation. Computational details are presented in the appendices.

II. HAMILTONIAN FORMALISM

We define the classical field ϕ as

$$\phi = \sigma(x - X(t), R(t)) + \chi(x - X(t), t) \; , \tag{2.1a}$$

where

$$\sigma(x,X,R) = \sigma_{\mathrm{SG}}\left[\frac{2\pi}{l_0}(x-X) + \mathcal{R}\right] - \sigma_{\mathrm{SG}}\left[\mathcal{R} - \frac{2\pi}{l_0}(x-X)\right] + \int_{\mathcal{R}}^{R} \psi_b(x - X, R')dR' \; . \tag{2.1b}$$

In (2.1b)

$$\sigma_{\mathrm{SG}}[x] = 4\tan^{-1}\exp x \tag{2.2a}$$

and ψ_b is the bound-state eigenfunction[20] of the linearized equation about the DSG static link.

Equation (2.1b) expresses the interesting fact that the DSG kink is a superposition of two sine-Gordon solitons. The last term in (2.1b) is introduced in order to have

$$\frac{\partial \sigma}{\partial R} = \psi_b(x - X, R) \tag{2.2b}$$

for all values of $\mathcal{R}$ even with $\chi = 0$. The requirement (2.2b) implies that when R is a function of t the DSG kink wobbles with a frequency related to the eigenfrequency of ψ_b. The nonlinear equation of motion for R has been derived in Ref. 11(b) within the framework of a constrained Hamiltonian formalism in which X, R, χ and their conjugate momenta P_x, P_R, and Π are treated as canonical variables. Also, in Ref. 11(b) we derive the equations of motion for the case where $\chi(x,t)$ depends on x and for the case where $\chi(x - X(t),t)$ depends on $x - X(t)$. The second case is preferable in the present problem because $X(t)$ becomes a cyclic variable. Also in Ref. 11(b) we obtain the equations of motion for $R(t)$ with the ansatz Eq. (2.1b). The fact that the exact bound state ψ_b appears in the ansatz has the important consequence in the present paper since ψ_b is orthogonal to the phonon modes the constraints Eq. (2.3b) mean simply that $\chi(x - X(t),t)$ and $\Pi(x - X(t),t)$ contain only DSG phonon modes.

Since the number of canonical variables in the single-soliton sector is increased by four the following four constraints need to be satisfied:

$$\int dx \frac{\partial \sigma}{\partial X}(x - X, R)\chi(x - X, t) = 0 \; , \qquad \int dx \frac{\partial \sigma}{\partial X}(x - X, R)\Pi(x - X, t) = 0 \; , \tag{2.3a}$$

$$\int dx \; \psi_b(x - X, R)\chi(x - X, t) = 0 \; , \qquad \int dx \; \psi_b(x - X, R)\Pi(x - X, t) = 0 \; , \tag{2.3b}$$

where the range of integration is $-\infty \to \infty$. Here,

$$\frac{\partial\sigma}{\partial X}=-\left[\frac{2\pi}{l_0}\right]\left[2\,\mathrm{sech}\left[\mathcal{R}+\frac{2\pi}{l_0}(x-X)\right]+2\,\mathrm{sech}\left[\mathcal{R}-\frac{2\pi}{l_0}(x-X)\right]\right]+\int_{\mathcal{R}}^{R}\frac{\partial\psi_b}{\partial X}(x-X,R')dR' . \tag{2.3c}$$

The function $(\partial\sigma/\partial X)(x-X,\mathcal{R})$ is the Goldstone mode[20] of the equations of the linearized phonons about the static DSG kink, while ψ_b is the shape mode.[20] The dimensionless Hamiltonian for the DSG single-kink sector is

$$H=\frac{1}{2\mathcal{D}}\left[M_{RR}\left[P_X+\int dx\,\Pi\chi'\right]^2+M_{XX}P_R^2-2M_{XR}\left[P_X+\int dx\,\Pi\chi'\right]P_R\right]+\tfrac{1}{2}\int\Pi^2dx+\tfrac{1}{2}\int dx[\chi'(x)+\sigma'(x)]^2$$
$$-\frac{8\pi}{l_0}(\cosh\mathcal{R})^{-2}\int dx\left\{\frac{1}{4}\sinh^2\mathcal{R}[\cos(\sigma+\chi)-1]-\left[1+\cos\left[\frac{\sigma+\chi}{2}\right]\right]\right\} . \tag{2.4}$$

The last integral in Eq. (2.4) is the DSG potential. Here P_X and P_R are the momenta conjugate to X and R and the prime denotes differentiation with respect to x. $\mathcal{D}$ is defined as

$$\mathcal{D}=M_{XX}M_{RR}-M_{XR}^2 , \tag{2.5a}$$

where

$$M_{XX}\equiv M_X\left[1-\frac{\langle\sigma''|\chi\rangle}{M_X}\right]^2+\frac{|\langle\psi_b'|\chi\rangle|^2}{M_R} , \tag{2.5b}$$

$$M_{RR}\equiv M_R\left[1-\frac{\langle\psi_{b,R}|\chi\rangle}{M_R}\right]^2+\frac{|\langle\psi_b'|\chi\rangle|^2}{M_X} , \tag{2.5c}$$

$$M_{XR}\equiv-\langle\psi_b'|\chi\rangle\left[2-\frac{\langle\sigma''|\chi\rangle}{M_X}-\frac{\langle\psi_{b,R}|\chi\rangle}{M_R}\right] . \tag{2.5d}$$

In Eq. (2.5) $\langle f|g\rangle\equiv\int f(x)g(x)dx$, and $\psi_{b,R}$ indicates differentiation with respect to R. M_X and M_R are defined as

$$M_X\equiv\langle\sigma'|\sigma'\rangle,\quad M_R\equiv|\langle\tilde{\psi}_b|f(R)\rangle|^2 \tag{2.6}$$

where the tilde on ψ_b indicates normalization to one and

$$f(R)\equiv2\,\mathrm{sech}\left[R+\frac{2\pi}{l_0}(x-X)\right]-2\,\mathrm{sech}\left[R-\frac{2\pi}{l_0}(x-X)\right] .$$

The superscript prime indicates derivative with respect to x. The potential in (2.4) depends on two-dimensionless parameters l_0 and $\mathcal{R}$. The parameter $l_0/2$ is roughly the size of a subkink of the DSG kink and the parameter $2\mathcal{R}$ is the equilibrium distance between the two subkinks of the DSG kink. A large value of l_0 corresponds to the situation in which the elastic energy represented by $(\partial\phi/\partial x)^2$ is larger than the underlying periodic potential energy. In Eq. (2.5) the kink solution σ depends on the dynamic variable R which varies between 0 and ∞.

In the following, we evaluate the DSG free energy within the harmonic approximation for the phonon field χ, by retaining only the quadratic terms in χ in a series expansion of the Hamiltonian (2.4) around the kink solution σ. We obtain

$$H=\frac{1}{2\mathcal{D}}\left[M_{RR}\left[P_X+\int dx\,\Pi\chi'\right]^2+M_{XX}P_R^2-2M_{XR}\left[P_X+\int dx\,\Pi\chi'\right]P_R\right]+v_{\mathcal{R}}(R)+V_1+V_2 , \tag{2.7a}$$

where

$$v_{\mathcal{R}}(R)\equiv\int dx\left\{\frac{1}{2}\left[\frac{\partial\sigma}{\partial X}\right]^2-\left[\frac{2\pi}{l_0}\right]^2\left[\tanh^2\mathcal{R}(\cos\sigma-1)-4(\cosh\mathcal{R})^{-2}\left[1+\cos\frac{\sigma}{2}\right]\right]\right\} , \tag{2.7b}$$

$$V_1\equiv\int dx\left\{\sigma'\chi'+\left[\frac{2\pi}{l_0}\right]^2\left[\tanh^2\mathcal{R}\sin\sigma-2(\cosh^2\mathcal{R})^{-2}\sin\left[\frac{\sigma}{2}\right]\right]\chi\right\}$$
$$\equiv\int dxS_{\mathcal{R}}(x)\chi(x) , \tag{2.7c}$$

$$V_2\equiv\int dx\left[\frac{1}{2}\chi'^2-\frac{\chi^2}{2}\left[\frac{2\pi}{l_0}\right]^2\left[-\tanh^2\mathcal{R}\cos\sigma+(\cosh\mathcal{R})^{-1}\cos\frac{\sigma}{2}\right]\right] . \tag{2.7d}$$

The term $v_{\mathcal{R}}(R)$ is the potential for the collective coordinate R in the absence of phonons, i.e., $\chi=0$.

For $\mathcal{R}_0>1.5$ [i.e., in the range of $\mathcal{R}$ where $\psi_b\approx f(R)$] both $v_{\mathcal{R}}(R)$ and $S(x)$ are easily evaluated analytically with the result that

$$v_{\mathcal{R}}(R)\rightarrow8\left[\frac{2\pi}{l_0}\right]\left[1+\frac{\tanh^2\mathcal{R}}{\tanh^2R}+2R\left[\frac{1}{\sinh2R}+\frac{\coth R}{\cosh^2\mathcal{R}}-\frac{\tanh^2\mathcal{R}\coth R}{2\sinh^2R}\right]\right] \tag{2.8}$$

and

$$S_{\mathcal{R}}(x)=-4\left[\frac{2\pi}{l_0}\right]^2\left[\left[\frac{\cosh R\,\sinh\left[\frac{2\pi}{l_0}x\right]}{\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}x\right]}\right](\mathrm{sech}^2\mathcal{R}-\mathrm{sech}^2 R)+\cosh R\,\sinh\left[\frac{2\pi}{l_0}x\right]\left[\frac{\cosh^2 R-\sinh^2\left[\frac{2\pi}{l_0}x\right]}{\left[\cosh^2 R+\sinh^2\left[\frac{2\pi}{l_0}x\right]\right]^2}\right](\tanh^2 R-\tanh^2\mathcal{R})\right]. \tag{2.9}$$

The rest energy of the DSG kink is then identified with

$$v_{\mathcal{R}}(\mathcal{R})=16\left[\frac{2\pi}{l_0}\right]\left[1+\frac{2\mathcal{R}}{\sinh 2\mathcal{R}}\right]. \tag{2.10}$$

In the following section we explicitly evaluate the single-kink partition function by integrating $e^{-\beta H}$ over the allowed phase space within the harmonic approximation for the phonon field χ. The free energy is then obtained in Sec. IV.

III. EVALUATION OF Z_1

In this section we shall evaluate Z_1, the canonical partition function in the single-soliton sector. For our constrained Hamiltonian system Z_1 is given by

$$Z_1=\int dR\,dP_R\,dX\,dP_X\,d\chi(x)\,d\Pi(x)\,\delta\left[\int dy\frac{\partial\sigma}{\partial X}\chi(y)\right]\delta\left[\int dy\frac{\partial\sigma}{\partial X}\Pi(y)\right]\delta\left[\int dy\,\psi_b\chi(y)\right]\delta\left[\int dy\,\psi_b\Pi(y)\right]e^{-\beta H}. \tag{3.1}$$

As required by the canonical formalism, the functional integration (3.1) has to include the constraints to obtain the proper restrictions on the available phase space. In (3.1) the R integration has to be performed last since the other integrations lead to results depending on R. Since $\mathcal{D}$ depends on χ it is necessary to perform the χ integration next to last.

In the following we shall compute Z_1 within the harmonic approximation for the phonon field χ in Eq. (2.7a). Note that, even if we retain the χ dependence only to second order in χ, the internal degrees of freedom represented by R can have very large anharmonic oscillations. This has been demonstrated in Ref. 21.

We perform the integrations over the canonical variables X, P_X, P_R, and χ. The integral over X gives L (the size of the system). The integrations over P_X and P_R give $(2\pi/\beta)\mathcal{D}^{1/2}(R,\chi)$ where $\mathcal{D}$ is the mass tensor. Being interested in condensed-matter physics applications, we treated the c.m. variable nonrelativistically:

$$Z_1=L\int dR\,d\chi\,d\Pi\left[\frac{2\pi}{\beta}\right]\mathcal{D}^{1/2}(R,\chi)\delta\left[\left\langle\frac{\partial\sigma}{\partial X}\middle|\chi\right\rangle\right]\delta\left[\left\langle\frac{\partial\sigma}{\partial X}\middle|\Pi\right\rangle\right]\delta\left[\langle\psi_b|\chi\rangle\right]\delta\left[\langle\psi_b|\Pi\rangle\right]\times e^{-\beta[v_{\mathcal{R}}(R)+V_1+V_2]}e^{-(\beta/2)\int\Pi^2dx}. \tag{3.2}$$

In Appendix A we perform the Π integration. The result [see Eq. (A5)] is

$$Z_\Pi\equiv\int d\Pi\,\delta\left[\left\langle\frac{\partial\sigma}{\partial X}\middle|\Pi\right\rangle\right]\delta(\langle\psi_b|\Pi\rangle)e^{-(\beta/2)\int\Pi^2dx}=\prod_{k=2}^{\infty}\left[\frac{2\pi}{\beta}\right]. \tag{3.3}$$

Upon substituting (3.3) in (3.2) we obtain

$$Z_1=L\left[\frac{2\pi}{\beta}\right]\prod_{k=2}^{\infty}\left[\frac{2\pi}{\beta}\right]\int dR\,\langle\mathcal{D}^{1/2}\rangle\int d\chi\,\delta\left[\left\langle\frac{\partial\sigma}{\partial X}\middle|\chi\right\rangle\right]\delta(\langle\psi_b|\chi\rangle)e^{-\beta[V_1+V_2+v_{\mathcal{R}}(R)]} \tag{3.4}$$

with

$$\langle\mathcal{D}^{1/2}\rangle\equiv\frac{\int\mathcal{D}^{1/2}(\chi)\delta(\langle(\partial\sigma/\partial x)|\chi\rangle)\delta(\langle\psi_b|\chi\rangle)e^{-\beta(V_1+V_2)}d\chi}{\int\delta(\langle(\partial\sigma/\partial X)|\chi\rangle)\delta(\langle\psi_b|\chi\rangle)e^{-\beta(V_1+V_2)}d\chi}. \tag{3.5}$$

The integration over the phonon variables gives [see Eq. (A12)]

$$Z_\chi = e^{-\beta\mathcal{E}_{\mathcal{R}}(R)} \prod_{k=2}^{\infty} \left[\frac{2\pi}{\beta}\right] \frac{1}{(\omega_k)^2} . \tag{3.6}$$

In (3.6) $\mathcal{E}_{\mathcal{R}}(R) \equiv -\sum_{k=2}^{\infty}(S_k^* S_k/\omega_k^2)$ is the kink self-energy arising from the V_1 term in Eq. (3.4). Finally Z_1 is written as

$$Z_1 = Z_{\text{phonon}} L \left[\frac{2\pi}{\beta}\right] e^{-\gamma} I(\mathcal{R},\gamma) , \tag{3.7}$$

where $\gamma \equiv E_K/kT$ and $E_K \equiv v_{\mathcal{R}}(\mathcal{R})$,

$$I(\mathcal{R},\gamma) = \int_0^\infty \langle \mathcal{D}^{1/2}(R) \rangle e^{-\beta\mathcal{E}_{\mathcal{R}}(R)} e^{-\beta[v_{\mathcal{R}}(R) - v_{\mathcal{R}}(\mathcal{R})]} dR \tag{3.8}$$

and

$$Z_{\text{phonon}} = \prod_{k=2}^{\infty} \left[\frac{2\pi}{\beta\omega_k}\right]^2 . \tag{3.9}$$

In Eq. (3.7) Z_{phonon} is the partition function of the phonons in the presence of a DSG kink. Following Rajaraman,[19] we write

$$Z_{\text{phonon}} = Z_0 \left[\frac{Z_{\text{phonon}}}{Z_0}\right] = Z_0 \frac{\prod_{k=-\infty}^{+\infty}{}'' \frac{2\pi}{\beta\omega_k}}{\prod_{k=-\infty}^{+\infty}{}'' \frac{2\pi}{\beta\hat{\omega}_k}}$$
$$\equiv Z_0 \exp\left[\sum_{-\infty}^{+\infty}{}'' \left[\ln\frac{\beta\hat{\omega}_k}{2\pi} - \ln\frac{\beta\omega_k}{2\pi}\right]\right] . \tag{3.10}$$

In (3.12) Z_0 is the partition function of the phonons in the absence of the kink and

$$\omega_k^2 = k^2 + \left[\frac{2\pi}{l_0}\right]^2, \quad kL + \Delta(k) = 2n\pi , \tag{3.11a}$$

while

$$\hat{\omega}_k^2 = k^2 + \left[\frac{2\pi}{l_0}\right]^2, \quad kL = 2n\pi . \tag{3.11b}$$

In (3.10) the prime on the product over k means to omit the discrete states $k=0$ and $k=1$. The $\hat{\omega}_k$ are the phonon frequencies in the absence of the DSG kink. The phonon density of states is defined as $dn(k)/dk$. From Eq. (3.11a) we get

$$\rho(k) \equiv \frac{dn(k)}{dk} = \frac{L}{2\pi} + \frac{1}{2\pi}\frac{d\Delta(k)}{dk} = \rho_0(k) + \frac{1}{2\pi}\frac{d\Delta(k)}{dk} \tag{3.12a}$$

and

$$\Delta\rho(k) \equiv \rho(k) - \rho_0(k) = \frac{1}{2\pi}\frac{d\Delta(k)}{dk} . \tag{3.12b}$$

From (3.11b) the density of states for the phonons in the absence of a kink is $\rho_0(k) = (L/2\pi)$. Taking the limit $L \to \infty$ leads to

$$Z_{\text{phonon}} = Z_0 \exp\left\{-\frac{1}{2\pi}\int_{-\infty}^{\infty} dk \frac{d\Delta(k)}{dk} \ln\left[k^2 + \left[\frac{2\pi}{l_0}\right]^2\right]^{1/2}\right\} \exp[\Delta(0_+)\pi^{-1}\ln(\beta/2\pi)]$$
$$\equiv Z_0 e^{-\theta(\mathcal{R})} \left[\frac{\beta}{2\pi}\right]^{(2+1/2)} . \tag{3.13}$$

The integrand in the exponent in Eq. (3.13) is independent of temperature and depends only on the parameters $\mathcal{R}$ and $(2\pi/l_0)$. The exact evaluation of $\Delta(k)$ and $\theta(\mathcal{R})$ is given in Appendix C.

We conclude this section by showing that $\mathcal{E}_{\mathcal{R}}$ is indeed the self-energy of the fluctuating source. For this purpose we observe that

$$-\mathcal{E}_{\mathcal{R}}(R) = \sum_{k=2}^{\infty} \frac{S_k^* S_k}{\omega_k^2}$$
$$= \sum_{k=2}^{\infty} \langle S|k\rangle \omega_k^{-2} \langle k|S\rangle$$
$$= \int S(x)\mathcal{G}[x,x']S(x)dx\,dx' , \tag{3.14}$$

where $\mathcal{G}$ is the static Green's function of the linearized DSG Schrödinger equation for χ and is defined by[11]

$$\frac{\partial^2 \mathcal{G}}{\partial t^2} + \mathcal{L}\mathcal{G} = (1 - \mathcal{P}_X - \mathcal{P}_R)1 , \tag{3.15}$$

where $\mathcal{P}_X$ and $\mathcal{P}_R$ are the projection operators for the constraints;[11] their role is to project out the discrete modes $|0\rangle = |(\partial\sigma/\partial X)\rangle$ and $|1\rangle = |\psi_b\rangle$ leaving only the phonon modes. Thus the time-dependent Green's function is

$$\mathcal{G}(\omega) = \sum_{k=2}^{\infty} |k\rangle \frac{1}{\omega_k^2 - \omega^2} \langle k| \tag{3.16}$$

and reduces to the static Green's function when $\omega = 0$. One can interpret Eq. (3.14) as the negative of the self-energy of the source distribution $S(X)$ in the field

$$\phi_{\text{stat}}(x) = \int \mathcal{G}[x,x']S(x')dx'$$

at point x produced by the source $S(x)$. The positive sign in the exponential of Eq. (A11) then represents the fact that the sum over k is the negative of the self-energy.

We can make the connection with the self-energy problem more explicit by evaluating $\mathcal{G}[x,x']$ for the static Klein-Gordon equation (i.e., we neglect the fact that the kink is present). We obtain

$$-\mathcal{E}_{\mathcal{R}}(R)=\sum_{k=2}\frac{S_k^* S_k}{\omega_k^2}$$
$$=\int S(x)e^{(-2\pi/l_0)|x-x'|}S(x')dx\,dx' . \quad (3.17)$$

In three dimensions the static Green's function is

$$(4\pi|x-x'|^{-1})\exp[-(2\pi/l_0)|x-x'|] ,$$

i.e., the Yukawa potential; in this context, $-\mathcal{E}_{\mathcal{R}}(\mathcal{R})$ is referred to as an "energy renormalization" or sometimes as a "mass renormalization." Here we shall refer to it as the "kink self-energy" because this term arises from the fluctuations of the internal variable R not the center-of-mass variable X.

IV. FREE ENERGY OF THE DILUTE GAS OF DSG KINKS

Currie *et al.*[5] showed how to go from phonon single-kink partition function, Z_1, to the grand-canonical partition function Ξ for any dilute-gas kink system. The partition function for N_1 kinks and N_2 antikinks is

$$\frac{(Z_{1K})^{N_1}}{N_1!}\frac{(Z_{1\bar{K}})^{N_2}}{N_2!}=\frac{(Z_1)^{N_1}}{N_1!}\frac{(Z_1)^{N_2}}{N_2!} , \quad (4.1)$$

where $\mathcal{Z}_1=Z_1/Z_0$.

In (4.1) the partition function for the single antikink, $\mathcal{Z}_{1K}$, is equal to the single-kink partition function $\mathcal{Z}_{1K}\equiv\mathcal{Z}_1$. The factorials $N_1!$ and $N_2!$ are required because the kinks and antikinks satisfy Boltzmann statistics.

In the following we assume the chemical potential of the kinks and antikinks to be the same. This assumption is not always allowed. For example, it is not valid when there is an external bias such as a mismatch between the period of the periodic potential and the period of the harmonic potential of the lattice. The grand-canonical partition function is then given by

$$\Xi=Z_0\sum_{N_1}\sum_{N_2}e^{\beta\mu N_1}\frac{\mathcal{Z}_1^{N_1}}{N_1!}e^{\beta\mu N_2}\frac{\mathcal{Z}_1^{N_2}}{N_2!}$$
$$=Z_0\exp(2e^{\beta\mu}\mathcal{Z}_1) , \quad (4.2)$$

where the factor 2 in Eq. (4.2) represents the fact that the kink and antikink have the same chemical potential and the same partition function. The free energy F is

$$F=-kT\ln\Xi=F^0-kT2e^{\beta\mu}\mathcal{Z}_1$$
$$=F^0-kTL2e^{\beta\mu}\left[\frac{\beta}{2\pi}\right]^{3/2}e^{-\Theta(\mathcal{R})}e^{-\gamma(\mathcal{R})}I(\gamma,\mathcal{R}) . \quad (4.3)$$

Here F^0 is the free energy of the phonon gas in the absence of the kink.

It is convenient to retain the chemical potential μ in the free energy; this allows, for example, the determination of the average kink number $\langle N\rangle$. μ is identically zero if there is no external constraint on the kink number. Using the definition $\langle N\rangle$ in terms of the grand-canonical free energy we obtain

$$-\left[\frac{\partial F}{\partial\mu}\right]_{T,L}=\langle N\rangle=2\mathcal{Z}_1 , \quad (4.4)$$

where $\mu=0$ in Eq. (4.4).

Recalling that the free energy F is given by $F=F_0-kT\langle N\rangle$, when $\mu=0$, we obtain the following expression for the free-energy density f

$$f=f^0-kT\langle n\rangle$$
$$=f^0-kT\left[2e^{-\Theta(\mathcal{R})}e^{-\gamma(\mathcal{R})}\left[\frac{\beta}{2\pi}\right]^{3/2}I(\gamma,\mathcal{R})\right] . \quad (4.5)$$

Equation (4.5) has to be compared with the conventional harmonic approximation. This we shall do in the next section.

V. INTERNAL-MODE CONTRIBUTION TO THE FREE ENERGY

In this section we determine the contribution of the collective variable R to the DSG kink free energy by evaluating the magnitude of $I(\gamma,\mathcal{R})$ in Eq. (3.8). We shall compare the free energy for the general case in which R undergoes nonlinear motion with the result of the harmonic-oscillator approximation where we replace the nonlinear potential $v_{\mathcal{R}}(R)-v_{\mathcal{R}}(\mathcal{R})$ with a potential quadratic in $(R-\mathcal{R})$. Further, we show that as $\mathcal{R}\to\infty$, the free energy reaches a constant value independent of $\mathcal{R}$.

For this purpose, using the harmonic approximation, valid when the potential for the R variable is quadratic, we show that the integral $I(\gamma,\mathcal{R})$ becomes

$$I=(2\pi M_X/\beta)^{1/2}\omega_0^{-1}(\mathcal{R}) . \quad (5.1)$$

Equation (5.1) is exactly the same result we would have obtained if we had not introduced R as a collective variable. [In other words, if at the beginning we had treated only X and P_X as collective variables so that χ included the internal oscillation $\psi_b(x)$ as well as the phonons we would have obtained exactly the harmonic-oscillator result Eq. (5.1).]

In order to obtain (5.1), we expand the exponential in Eq. (3.8) for $I(\gamma,\mathcal{R})$ to second order in $\rho\equiv R-\mathcal{R}$

$$v_{\mathcal{R}}(R)-v_{\mathcal{R}}(\mathcal{R})=\tfrac{1}{2}M_R(\mathcal{R})\omega_0^2(\mathcal{R})\rho^2 , \quad (5.2)$$

where we have neglected the contribution of $\mathcal{E}_{\mathcal{R}}(R)$ which we have calculated to be less than one percent of the right-hand side of Eq. (5.2). In the harmonic-oscillator limit M_X and M_R are to be evaluated at $R=\mathcal{R}$, consequently as shown in Appendix B

$$\langle\mathcal{D}^{1/2}\rangle=[M_X(\mathcal{R})M_R(\mathcal{R})]^{1/2} .$$

Thus,

$$I(\gamma,\mathcal{R})=[M_X(\mathcal{R})M_R(\mathcal{R})]^{1/2}\times\int_{-\infty}^{\infty}d\rho\, e^{-(1/2\beta M_{\mathcal{R}}(\mathcal{R})\omega_0^2(\mathcal{R})\rho^2}d\rho$$
$$=M_X^{1/2}(\mathcal{R})\left[\frac{2\pi}{\beta\omega_0^2(\mathcal{R})}\right]^{1/2}. \quad (5.3)$$

Next we show that the values of $\rho\equiv R-\mathcal{R}$ which contribute to the DSG kink free energy are sufficiently large that the collective variable R must be treated as a nonlinear oscillator. The values of ρ which contribute are those for which $\frac{1}{2}M_{\mathcal{R}}\omega_0^2\rho^2\sim kT$. Dividing this equation by M_X leads to

$$\frac{1}{2}\frac{M_R}{M_X}\omega_0^2\rho^2=\tfrac{1}{2}g(\mathcal{R})\rho^2=\frac{kT}{M_X}\equiv\frac{kT}{E_K}. \quad (5.4)$$

For $R>1.25$, $g(\mathcal{R})$ [see Ref. 11(a)] is

$$g(\mathcal{R})=\left[\frac{\sinh(2\mathcal{R})}{\sinh(2\mathcal{R})+2\mathcal{R}}\right]\left[\frac{(3-\mathcal{R}\coth\mathcal{R})}{\sinh^2\mathcal{R}}+\frac{\mathcal{R}\tanh\mathcal{R}-1}{\cosh^2\mathcal{R}}-\frac{2\mathcal{R}\coth\mathcal{R}}{\cosh^2\mathcal{R}\sinh^2\mathcal{R}}\right]. \quad (5.5)$$

Notice that the quantity (kT/E_K) is the small parameter which justifies the dilute DSG kink approximation. Thus, for a typical value of $kT/E_K=\frac{1}{5}$ and width $\mathcal{R}\sim 3$ one finds that $\rho\geq 2$. Thus, the variations in R lie in a range where the harmonic approximation is not valid.

We determine the contribution of the nonlinearity of the R variable to the free energy by evaluating Eq. (5.1) numerically and comparing the outcome of the numerical integration with the result of the harmonic-oscillator (HO) approximation. For this purpose we compute the ratio

$$\frac{(f-f_0)_{\rm HO}}{(f-f_0)}=\frac{\langle n\rangle_{\rm HO}}{\langle n\rangle}=\left[\frac{2\pi M_X}{\beta}\right]^{1/2}\omega_0^{-1}(\mathcal{R})[I(\gamma,\mathcal{R})]^{-1}. \quad (5.6)$$

Equation (5.6) is valid for all $\mathcal{R}$. The region where $\mathcal{R}>1.25$ is the region where the nonlinear variation in R is most important. In this region we produced in the previous sections analytic expressions for $M_{\mathcal{R}}(R)$, $M_X(R)$, $v_{\mathcal{R}}(R)$, $\omega_0(\mathcal{R})$, and $S_{\mathcal{R}}(x,R)$. Consequently, we are able to perform the integration in Eq. (5.6) numerically for $\mathcal{R}>2$ using our analytic expressions for the functions appearing in $I(\gamma,\mathcal{R})$. We present the results in Fig. 1. The large deviations of the ratio $(f-f_0)_{\rm HO}/(f-f_0)$ from one indicates that the dominant contribution to the collective variable R to the DSG kink free energy comes from the nonlinear motion of R. For the entire range of $v_{\mathcal{R}}$ we find that $\mathcal{E}_{\mathcal{R}}(R)$ is less than one percent of $v_{\mathcal{R}}(R)$ so that the kink self-energy contribution is small compared with the bare nonlinear oscillation of the collective variable R in the potential $v_{\mathcal{R}}(R)$. For the important range of values of $\mathcal{R}$ around 3 the contribution of the collective variable R to the DSG kink free energy is two to three times larger than that given by the harmonic-oscillator approximation. The cause of the $\mathcal{R}$ dependence of the free-energy ratio $(f-f_0)_{\rm HO}/(f-f_0)$ is that even though the curvature of the harmonic-oscillator potential and the full nonlinear potential [neglecting the less than one percent contribution from $\mathcal{E}_{\mathcal{R}}(R)$] are the same, namely $M_R(\mathcal{R})\omega_0^2(\mathcal{R})$ the potential $v_{\mathcal{R}}(R)$ depends explicitly[11] on $\mathcal{R}$. For $\mathcal{R}>5$ we see that the harmonic-oscillator free energy becomes increasingly larger than the correct nonlinear free energy. The reason for this is that the harmonic-oscillator free energy is proportional to $[\omega_0(\mathcal{R})]^{-1}$ and $\omega_0(\mathcal{R})$ goes to zero for large $\mathcal{R}$ as $e^{-2\mathcal{R}}$. However, the nonlinear oscillator's effective frequency is strongly amplitude dependent and it is much

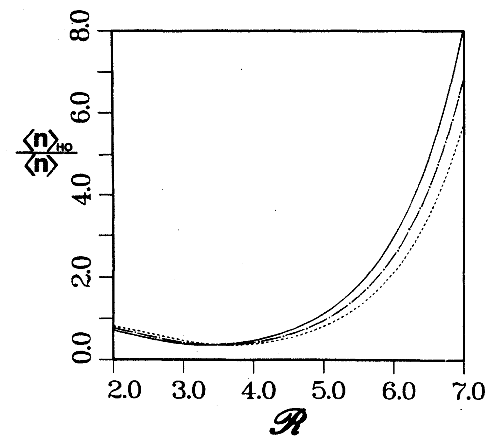

FIG. 1. A plot of the ratio $(f-f_0)_{\rm HO}/(f-f_0)$ as a function of $\mathcal{R}$ for $\gamma=10$ (dotted line), $\gamma=7$ (dot-dashed line), and $\gamma=5$ (solid line).

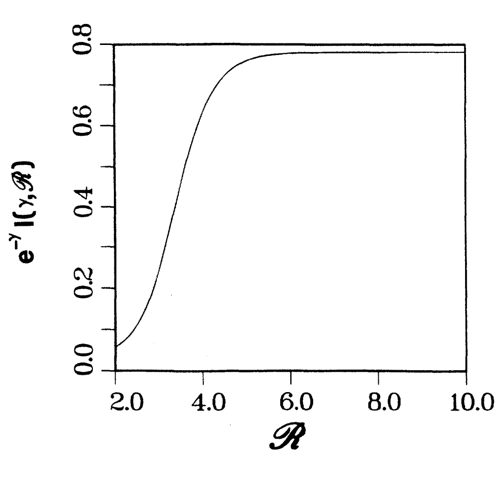

FIG. 2. The function $e^{-\gamma}I(\gamma,\mathcal{R})$ vs $\mathcal{R}$ for $\gamma=7$.

smaller than $\omega_0(\mathcal{R})$ for large $\mathcal{R}$. In fact, as we see from Fig. 2, the free energy as $\mathcal{R}\rightarrow\infty$ approaches a limit independent of $\mathcal{R}$. The reason why the free energy becomes independent of $\mathcal{R}$ at large $\mathcal{R}$ is that $v_{\mathcal{R}}(R)$, $M_R(\mathcal{R})$, and $M_X(\mathcal{R})$ are well behaved and become independent of $\mathcal{R}$ as $\mathcal{R}\rightarrow\infty$. The resultant R integrand is then well behaved for all R and approaches $\exp(-2R)$ as $R\rightarrow\infty$.

The results of this section demonstrate the need for including the nonlinear motion of the collective variable R in the equilibrium statistical mechanics of DSG systems. Effects coming from the nonlinear motion of the R variable are expected to be relevant in the analysis of magnetic systems modeled by the DSG theory.[16]

VI. CONCLUSIONS

In this paper we analyzed the equilibrium statistical mechanics of a dilute gas of DSG kinks including the effects of the internal nonlinear oscillatory degree of freedom characteristic of this system. Our approach used the path-integral method developed in Ref. 19.

Using the results of Refs. 11 and 20 we derived the free energy as a function T and $\mathcal{R}$. In fact, our solution of the linearized Schrödinger equation for the DSG system enabled us to evaluate the phase shift $\Delta(k)$ of the phonon modes in the presence of the DSG kink. This provided us with the density of states in the one soliton sector. Our expression for $\Delta(k)$ is compatible with Levinson's theorem, for all finite values of $\mathcal{R}$. Furthermore, our Hamiltonian treatment[11] of the wobbling motion of the DSG kink allowed us to include the anharmonic effects in the motion of the associated dynamical variable $R(t)$. These nonlinear effects are manifest in the term $I(\gamma,\mathcal{R})$ defined in the text.

We have compared the free energy obtained by considering the full anharmonic motion of the R variable with that corresponding to the harmonic approximation in R. The results of this comparison are plotted in Fig. 1 and discussed in Sec. V.

In Ref. 21, we showed that when the equations of motion for $R(t)$ in the potential $v_{\mathcal{R}}(R)$ were solved for $R(t)$ and the results substituted into $\sigma(x-X(t),R(t))$ we obtained very good agreement with molecular dynamics simulations both for the frequencies (within 1% or 2%) and for the shape mode of the DSG kink. The agreement with simulations continued to be good even when the nonlinearity was sufficiently large that the frequency of oscillation depended appreciably on amplitudes. The agreement was remarkable in that we had set $\chi=0$, i.e., neglected the phonons which was consistent with the simulations where the radiation of phonons was very small in many parameter ranges. The reason that there is weak radiation of phonons even for appreciable nonlinear oscillations of R is that the frequency of the R motion is below the frequency of the phonon modes which start at $\omega=(2\pi/l_0)$, e.g., at $\mathcal{R}=2$ we have $\omega_0=0.36(2\pi/l_0)$. Consequently, the third harmonic of the motion of $R(t)$ is the first harmonic to radiate. As $\mathcal{R}$ increases even higher harmonics are required in order that phonons are radiated. On the other hand, as $\mathcal{R}$ decreases, the second harmonic radiates and the condition that we retain only quadratic terms in χ puts limits on the degree of nonlinearity in R motion which is consistent with our initial assumptions. In summary, for larger $\mathcal{R}$ we have large nonlinear motion of R with χ very small. The nonlinearity consists of two types of contributions: nonradiative and radiative. By nonradiative we mean the motion is nonlinear but the higher harmonics which are resonant with phonons, $m\omega_0>(2\pi/l_0)$, are so weak that radiation is very small. Thus, the effect of the nonlinear phonons is the dressing of the kink. On the other hand, as the nonlinearity increases the higher harmonics will become large enough to radiate and phonons will be radiated. The approximations in this paper are valid when the radiated phonons can be treated as quadratic in χ. In equilibrium statistical thermodynamics we do not directly see the dynamical phonon absorption and emission processes. The only indirect measure of these processes is in the quantity $I(\gamma,\mathcal{R})$ appearing in the DSG kink free energy.

We neglected the interaction between kinks. In order to include their effect, one should compute[22] the scattering cross section for the collision of two kinks. The presence of resonances,[8] as well as the possibility of radiation of phonons, makes this computation particularly interesting in this model. Moreover, once the interaction between kinks is included in the partition function, one should be able to analyze in greater detail the phase transitions induced[16] by pairing the kinks in realistic condensed-matter systems modeled by an effective one-dimensional DSG theory.

Finally, an analysis similar to the one carried out in this paper for the DSG theory is possible[23] also for the ϕ^4 model, when the contribution of wobblers to the partition function is taken into account. The existence of wobbling kinks for the ϕ^4 theory has been proved in Ref. 24.

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APPENDIX A: THE Π AND χ INTEGRATIONS

We first show that the integration over $\Pi(x)$ in Eq. (3.2) yields (3.3). In Ref. 20 we solved the eigenvalue problem for the linearized phonons in the presence of a DSG static kink. The equation has the Schrödinger form

$$\mathcal{L}|k\rangle=\omega_k^2|k\rangle \tag{A1}$$

with

$$|0\rangle\equiv\left|\frac{\partial\sigma_{\mathrm{DSG}}}{\partial X}\right\rangle,\quad |1\rangle\equiv|\psi_b\rangle\ ,$$

where

$$\frac{\partial\sigma_{\rm DSG}}{dX}=-\left[\frac{4\pi}{l_0}\right]\left[\operatorname{sech}\left[R+\frac{2\pi}{l_0}(x-X)\right]\right.$$
$$\left.+\operatorname{sech}\left[R+\frac{2\pi}{l_0}(x-X)\right]\right],$$

being the discrete modes and the eigenstates $|k\rangle$ for $k=-\infty,\ldots,-2,2,\ldots\infty$. The functions $\langle x|\psi_b\rangle=\psi_b(x)$ and $\langle x|k\rangle=\psi_k(x)$ are given in Ref. 20 and in Appendix C. The set $|k\rangle$ is a complete orthonormal set of functions[20] which we shall use as a basis (k basis) for expanding $|\Pi\rangle$ so that

$$|\Pi\rangle=p_0|0\rangle+p_1|1\rangle+\sum_{k=-\infty}^{\infty}{}''p_k|k\rangle\ . \tag{A2}$$

In Eq. (A2) p_0 and p_1 are real while p_k for $k\neq 0$ are complex. The double prime on the summation denotes the omission of the two discrete states $|0\rangle$ and $|1\rangle$. Since $\Pi(x)$ is real one has $p_{-k}=p_k^*$. The two Π constraints are thus

$$\delta\left[\int dy\frac{\partial\sigma}{\partial X}\Pi(y)\right]=\delta(\langle\Pi|0\rangle)=\delta\left[p_0+\sum_{-\infty}^{\infty}{}''C_kp_k\right], \tag{A3a}$$

$$\delta\left[\int dy\,\psi_b\Pi(y)\right]=\delta(\langle\Pi|1\rangle)=\delta(p_1)\ . \tag{A3b}$$

where C_k is defined below. The integral of $\Pi^2(x)$ is then

$$\int\Pi^2(x)dx=\langle\Pi|\Pi\rangle=p_0^2+p_1^2+\sum_{-\infty}^{\infty}{}''p_k^*p_k\ . \tag{A4}$$

Substituting Eqs. (A3a), (A3b), and (A4) in Eq. (A1) yields

$$Z_\pi=\int dp_0dp_1\prod_{k=2}^{\infty}2dp_k^rdp_k^i\delta\left[p_0+2\sum_{k=2}^{\infty}(C_k^rp_k^r+C_k^ip_k^i)\right]\delta(p_1)\exp\left[-\frac{\beta}{2}\left[p_0^2+p_1^2+2\sum_{k=2}^{\infty}[(p_k^r)^2+(p_k^i)^2]\right]\right]$$
$$=[1+\alpha]^{-1/2}\prod_{k=2}^{\infty}\left[\frac{2\pi}{\beta}\right], \tag{A5}$$

where

$$\alpha\equiv\sum_{k'=2}^{\infty}|C_{k'}|^2=\sum_{k'=2}^{\infty}\left|\left\langle k'\left|\frac{d\hat\theta}{dX}\right.\right\rangle\right|^2$$

and where

$$\hat\theta=\int_{\mathcal{R}}^{R}\left[\psi_b(x-X,R')-\frac{d\sigma_{\rm DSG}}{dR'}(x-X,R')\right]dR'\ .$$

The quantity α is independent of temperature and approaches zero for $\mathcal{R}$ greater than one. For example, for $\mathcal{R}\gtrsim 1.5$, $\alpha\lesssim 0.01$. Consequently, for convenience we will neglect α in Eq. (A5) in the present paper. In Eq. (A5) we expressed the complex p_k in terms of its real and imaginary parts p_k^r and p_k^i. Consequently, in the p_k^r,p_k^i representation k goes over only positive values. This implies that there is a factor of $(2\pi/\beta)^{1/2}(2\pi/\beta)^{1/2}$ for each k. When V_1 is absent in the Hamiltonian Eq. (2.8) the integration over χ leads to the phonon potential-energy contribution

$$Z_\chi=\prod_{k=2}^{\infty}\left[\frac{2\pi}{\beta}\right]\frac{1}{\omega_k^2}\ . \tag{A6}$$

We now show that the effect of V_1—which is linear in χ—causes each phonon oscillator to oscillate about a center displaced from the origin.

The integral over χ in Eq. (3.4) is

$$Z_\chi\equiv\int\delta\left[\left\langle\frac{\partial\sigma}{\partial X}\right|\chi\left.\right\rangle\right]\delta(\langle\psi_b|\chi\rangle)e^{-\beta(V_1+V_2)}d\chi(x)\ . \tag{A7}$$

When we expand $|\chi\rangle$ and $|S\rangle$ in terms of the eigenfunction of the operator $\mathcal{L}$ we obtain

$$|\chi\rangle=q_0|0\rangle+q_1|1\rangle+\sum_{k=-\infty}^{\infty}{}''q_k|k\rangle\ , \tag{A8a}$$

$$|S\rangle=S_0|0\rangle+S_1|1\rangle+\sum_{k=-\infty}^{\infty}{}''S_k|k\rangle\ , \tag{A8b}$$

where q_0, q_1, S_0, and S_1 are real. Since $|\chi\rangle$ and $|S\rangle$ are real we have $q_{-k}=q_k^*$ and $S_{-k}=S_k^*$. In the k basis the δ functions in Eq. (A7) are

$$\delta\left[\left\langle\chi\left|\frac{\partial\sigma}{\partial X}\right.\right\rangle\right]=\delta\left[q_0+2\sum_{k=2}^{\infty}(C_k^rq_k^r+C_k^iq_k^i)\right],$$
$$\delta(\langle\chi|\psi_b\rangle)=\delta(q_1) \tag{A9}$$

while V_1 and V_2 are given by

$$V_1=\langle\chi|S\rangle=q_1S_1+2\sum_{k=2}^{\infty}(q_k^rS_k^r+q_k^iS_k^i)\ , \tag{A10a}$$

$$V_2=\tfrac{1}{2}\langle\chi|\mathcal{L}|\chi\rangle$$
$$=\tfrac{1}{2}\omega_1^2q_1^2+\sum_{k=2}^{\infty}\omega_k^2[(q_k^r)^2+(q_k^i)^2]\ . \tag{A10b}$$

Thus,

$$\exp[-\beta(V_1+V_2)]=\exp\left[\beta\left[\frac{1}{2}\frac{S_1^2}{\omega_1^2}+\sum_{k=2}^{\infty}\frac{S_k^*S_k}{\omega_k^2}\right]\right]\exp\left[-\frac{\beta}{2}\omega_1^2\left[q_1+\frac{S_1}{\omega_1^2}\right]^2\right]$$
$$\times\exp\left\{-\beta\sum_{k=2}^{\infty}\omega_k^2\left[\left[q_k^r+\frac{S_k^r}{\omega_k^2}\right]^2+\left[q_k^i+\frac{S_k^i}{\omega_k^2}\right]^2\right]\right\}. \tag{A11}$$

Upon substituting Eqs. (A9) and (A11) in Eq. (A7) we obtain

$$Z_\chi=\exp\left[\beta\sum_{k=2}\frac{S_k^*S_k}{\omega_k^2}\right]\prod_{k=2}^{\infty}\int 2\,dq_k^r dq_k^i\exp\left\{-\beta\omega_k^2\left[\left[q_k^r+\frac{S_k^r}{\omega_k^2}\right]^2+\left[q_k^i+\frac{S_k^i}{\omega_k^2}\right]^2\right]\right\}$$
$$=\exp[-\beta\mathcal{E}_{\mathcal{R}}(R)]\prod_{k=2}^{\infty}\left[\frac{2\pi}{\beta}\right]\frac{1}{\omega_k^2} \tag{A12}$$

which is Eq. (3.6) of the text.

APPENDIX B

The purpose of this appendix is to show that $\langle\mathcal{D}^{1/2}\rangle$ is approximately equal to $(M_X M_R)^{1/2}$. We shall evaluate $\mathcal{D}$ within the harmonic approximation in χ used in this paper. From Eq. (2.6) we obtain

$$\mathcal{D}\approx M_X(1-b)^2M_R(1-c)^2+|\langle\psi_b'|\chi\rangle|^2\left[(1-b)^2+(1-c)^2-(2-b-c)^2+\frac{|\langle\psi_b'|\chi\rangle|^2}{M_X M_R}\right]$$
$$=M_X(1-b)^2M_R(1-c)^2-2|\langle\psi_b'|\chi\rangle|^2\left[(1-b)(1-c)-\frac{1}{2}\frac{|\langle\psi_b'|\chi\rangle|^2}{M_X M_R}\right], \tag{B1}$$

where

$$b\equiv\frac{\langle\sigma''|\chi\rangle}{M_X}$$

and

$$c\equiv\frac{\langle\psi_{b,R}|\chi\rangle}{M_R}.$$

Averaging the term $|\langle\psi_b'|\chi\rangle|^2$ over χ leads to

$$\langle|\langle\psi_b'|\chi\rangle|^2\rangle=2kT\langle\psi_b'|\mathcal{G}|\psi_b'\rangle .$$

Consequently since (kT/M_X) is our small parameter we can neglect the $|\langle\psi_b'|\chi\rangle|^2$ in Eq. (B1). When we take the square root of Eq. (B1) and average over χ we obtain

$$\langle\mathcal{D}^{1/2}\rangle\approx(M_X M_R)^{1/2}\langle(1-b)(1-c)\rangle$$
$$\approx(M_X M_R)^{1/2}\langle 1-b-c\rangle . \tag{B2}$$

Note that the $\langle bc\rangle$ term is proportional to (kT/M_X). The terms $\langle b\rangle$ and $\langle c\rangle$ are nonzero because

$$\langle b\rangle=\frac{\langle\sigma''|\mathcal{G}|S\rangle}{M_X}\quad\text{and}\quad\langle c\rangle=\frac{\langle\psi_{b,R}|\mathcal{G}|S\rangle}{M_R}$$

due to the V_1 term. However, they are independent of temperature and make only a negligible contribution to the R dependence of $\langle\mathcal{D}^{1/2}\rangle$.

Neglecting $\langle b\rangle$ and $\langle c\rangle$ one can replace $\langle\mathcal{D}^{1/2}\rangle$ by $[M_X(R)M_R(R)]^{1/2}$. However, the R dependence of $\langle\mathcal{D}^{1/2}\rangle$ makes a contribution to the R integration.

APPENDIX C: PHASE SHIFT AND LEVINSON'S THEOREM

In this appendix, we evaluate $\Delta(k)$ and $\Theta(\mathcal{R})$. Our computation relies heavily on the results of Ref. 20. There, we noticed that the Schrödinger equation describing the linearized dynamics of the phonons in the presence of a single DSG kink is the supersymmetric partner of a modified Pöschl-Teller (PT) equation and were able to provide the complete set of eigenfunctions. Here, we use supersymmetry to evaluate the phase shift of the linearized phonons.

We shall use $\psi(x)$ to denote the phonons modes in the presence of the DSG kink and we will use $\varphi(x)$ to denote the eigenfunctions of the Pöschl-Teller Hamiltonian. Supersymmetry gives

$$\psi(x)\equiv D\varphi(x)=\left[\frac{d}{dx}+W(x)\right]\varphi(x) , \tag{C1a}$$

where[20]

$$W(x)=\tanh\left[\frac{2\pi x}{l_0}+\mathcal{R}\right]+\tanh\left[\frac{2\pi x}{l_0}-\mathcal{R}\right]$$
$$-\tanh\left[\frac{2\pi x}{l_0}\right]. \tag{C1b}$$

The spectrum of the linearized phonon modes of the PT Hamiltonian is then given by a bound state, and a continuum starting at $\omega_m^2=(2\pi/l_0)^2$ with eigenfunctions

$$\varphi(x)=A\varphi_k^e(x)+b\varphi_k^0(x) . \tag{C2}$$

Equation (C2) is a linear combination of even and odd standing wave functions, which diagonalize simultaneously the eigenfunctions of the Hamiltonian and the parity operator. The unnormalized eigenfunctions are[25]

$$\varphi_k^e=\cosh^s(\alpha x)\,{}_2F_1[a,b,\tfrac{1}{2};-\sinh^2(\alpha x)]$$
$$=\frac{\cosh[(2a-1)\alpha x]}{\cosh^{1-s}(\alpha x)} \tag{C3a}$$

and

$$\varphi_k^0=\cosh^s(\alpha x)\sinh(\alpha x)\,{}_2F_1[a+\tfrac{1}{2},b+\tfrac{1}{2};\tfrac{3}{2};-\sinh^2(\alpha x)]$$
$$=\frac{\sinh[(2a-1)\alpha x]}{(2a-1)\cosh^{1-s}(\alpha x)} \,. \tag{C3b}$$

In Eqs. (C3)

$$a=\frac{1}{2}\left[s+\frac{ik}{\alpha}\right], \tag{C4a}$$

$$b=\frac{1}{2}\left[s-i\frac{k}{\alpha}\right], \tag{C4b}$$

where $k^2=\omega^2-(2\pi/l_0)^2$ and

$$\alpha=\left[\frac{2\pi}{l_0}\right]\tanh^2\mathcal{R}\frac{\sinh 2\mathcal{R}}{\sinh 2\mathcal{R}-2\mathcal{R}}\,, \tag{C5a}$$

$$s=\frac{1}{2}\left[-1+\left[1+\frac{8\tanh^2\mathcal{R}}{\alpha^2}\right]^{1/2}\right]. \tag{C5b}$$

We introduce the scattering solutions of the Pöschl-Teller Hamiltonian as

$$\varphi(x)=\begin{cases}(e^{ikx}-R_{\rm PT}e^{-ikx}), & x\to-\infty\,,\\ T_{\rm PT}e^{ikz}, & x\to\infty\,.\end{cases} \tag{C6}$$

Similarly, the scattering eigenfunctions of the linear phonons in the presence of the DSG kink are given by

$$\psi(x)=\begin{cases}(e^{ikx+i\delta}+{\rm R}e^{-ikx+i\delta}), & x\to-\infty\,,\\ Te^{ikx+i\delta}, & x\to\infty\,,\end{cases} \tag{C7}$$

where $\delta\equiv\delta(k,\mathcal{R})$ is an overall constant phase.

Supersymmetry relates (C6) and (C7). For $x\to\infty$ we have

$$\frac{R}{R_{\rm PT}}=\frac{1-ik}{1+ik}e^{i\delta} \tag{C8}$$

which, in turn, leads to

$$\Delta=\Delta_{\rm PT}+\delta-2\arctan k\,. \tag{C9}$$

In (C9) Δ and $\Delta_{\rm PT}$ are the phase shifts of the two supersymmetric partner Hamiltonians. From Ref. 20 one gets

$$\Delta_{\rm PT}(k,\mathcal{R})=-\left[\Delta_e(k,\mathcal{R})+\Delta_0(k,\mathcal{R})+\frac{\pi}{2}\right] \tag{C10a}$$

with

$$\Delta_e=\arg\frac{\Gamma\left[\dfrac{ik}{\alpha}\right]\exp(-k\ln 2/\alpha)}{\Gamma\left[\dfrac{s}{2}+\dfrac{ik}{2\alpha}\right]\Gamma\left[\dfrac{1-s}{2}+\dfrac{ik}{2\alpha}\right]} \tag{C10b}$$

and

$$\Delta_0=\arg\frac{\Gamma\left[\dfrac{ik}{\alpha}\right]\exp(-ik\ln 2/\alpha)}{\Gamma\left[\dfrac{s-1}{2}+\dfrac{ik}{2\alpha}\right]\Gamma\left[1+\dfrac{s}{2}+\dfrac{ik}{2\alpha}\right]}\,. \tag{C10c}$$

In (C10) Δ_e (Δ_0) is the phase shift of the even (odd) standing wave functions of the Pöschl-Teller Hamiltonian.

We shall now evaluate $\Delta_{\rm PT}(k,\mathcal{R})$. Use of (C10b) and (C10c) and of

$$\Gamma(z)\Gamma(1-z)=\frac{\pi}{\sin\pi z}$$

leads to

$$\Delta_e(k,\mathcal{R})+\Delta_0(k,\mathcal{R})=2\arg\frac{\Gamma\left[\dfrac{ik}{\alpha}\right]\exp(-ik\log_{10}2/\alpha)}{\Gamma\left[\dfrac{s}{2}+\dfrac{ik}{2\alpha}\right]\Gamma\left[\dfrac{s}{2}+\dfrac{1}{2}+\dfrac{ik}{2\alpha}\right]}$$
$$-\arg\left[\sin\pi\left[\frac{s}{2}+\frac{1}{2}+\frac{ik}{2\alpha}\right]\right]$$
$$-\arg\left[\sin\pi\left[\frac{s}{2}+\frac{ik}{2\alpha}\right]\right]. \tag{C11}$$

Finally, use of the product formula

$$\prod_{J=0}^{n-1}\Gamma\left[z+\frac{J}{n}\right]=(2\pi)^{(n-1)/2}n^{(1/2)-nz}\Gamma(nz)$$

and a reshaping of the last two terms in the right-hand side of Eq. (C11) gives

$$\Delta_{\rm PT}(k,\mathcal{R})=-2\arg\frac{\Gamma\left[\dfrac{ik}{\alpha}\right]}{\left[s+\dfrac{ik}{\alpha}\right]}$$
$$+\arctan\left[\cot\pi s\,\tanh\pi\frac{k}{\alpha}\right]-\frac{\pi}{2}\,. \tag{C12}$$

Equation (C12) is consistent with Levinson's theorem for any finite $\mathcal{R}$. Equations (C9) and (C12) imply

$$\Delta(k,\mathcal{R})=2\pi\mathrm{sgn}k-2\arctan k+\arctan\left[\cot\pi s\tanh\pi\frac{k}{\alpha}\right]-2\arg\frac{\Gamma\left[\frac{ik}{\alpha}\right]}{\Gamma\left[s+\frac{ik}{\alpha}\right]}-\frac{\pi}{2}\,. \tag{C13}$$

In (C13) the global overall phase $\delta(k,\mathcal{R})$ has been put equal to $2\pi\mathrm{sgn}k$ to give $\Delta(\infty,\mathcal{R})=0$ for any finite $\mathcal{R}$. Again, Levinson's theorem in satisfied. In fact,

$$\Delta(0_+)=(2+\tfrac{1}{2})\pi \tag{C14}$$

for any $\mathcal{R}$.

Equation (C14) states that the spectrum of the linearized phonons in the presence of a static DSG kink admits two bound states. This is consistent with results of previous analysis.[8,10,20] The factor $\frac{1}{2}$ in (C14) arises[26] because the Jost function vanishes at $k=0$.

Finally, we evaluate

$$\Theta(\mathcal{R})\equiv\frac{1}{2\pi}\int_{-\infty}^{+\infty}dk\frac{d\Delta}{dk}\ln\left[k^2+\left[\frac{2\pi}{l_0}\right]^2\right]^{1/2}. \tag{C15}$$

Integration by parts leads to

$$\Theta(\mathcal{R})=-\frac{1}{2\pi}\int_{-\infty}^{+\infty}dk\frac{k\Delta(k)}{k^2+\left[\frac{2\pi}{l_0}\right]^2} \tag{C16}$$

so that only the odd terms of (C9) contribute to (C16). Use of the residue theorem gives then

$$\Theta(\mathcal{R})=2\pi\left\{\operatorname{arctanh}\left[\frac{2\pi}{l_0}\right]-\tfrac{1}{2}\operatorname{arctanh}\left[\cot(\pi s)\tan\left[\frac{2\pi}{\alpha l_0}\right]\right]-\pi\right\}. \tag{C17}$$

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[1]A. R. Bishop, J. A. Krumhansl, and S. E. T. Trullinger, Physica **1D**, 1 (1980); K. Maki, in *Electronic Properties of Inorganic Quasi-One-Dimensional Materials,* edited by P. Monceau (Reidel, Dortrecht, 1985).

[2]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B **11**, 3535 (1975).

[3]D. J. Scalapino, M. Sears, and R. A. Farrell, Phys. Rev. B **6**, 3409 (1972).

[4]See, for example, J. F. Currie, M. B. Fogel, and F. L. Palmer, Phys. Rev. A **16**, 796 (1977); K. R. Sabbaswamy and S. E. Trullinger, *ibid.* **19**, 1340 (1979); F. F. Currie, S. Serkeve, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **20**, 2213 (1979); A. R. Bishop, Physica **93a**, 82 (1978); in *Solitons in Condensed Matter Physics,* edited by A. R. Bishop and T. Schneider (Springer-Verlag, Berlin, 1978); N. Gupta and B. Sutherland, Phys. Rev. A **14**, 1790 (1976); S. E. Trullinger, Phys. Rev. B **22**, 4558 (1980).

[5]J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).

[6]N. Theodorakopoulos, Z. Phys. B **46**, 367 (1982); K. Sasaki, Phys. Rev. B **33**, 2214 (1986).

[7]P. Sodano, in *Quantum Field Theory,* edited by F. Mancini (North-Holland, Amsterdam, 1986); R. K. Bullough, P. J. Caudrey, and H. M. Gibbs, in *Solitons,* edited by R. K. Bullough and P. J. Caudrey (Springer-Verlag, Berlin, 1980); R. K. Bullough and P. J. Caudrey, in *Nonlinear Evolution Equations Solvable by the Spectral Transform,* edited by F. Calogero (Pitman, London, 1978).

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

[9]C. A. Condat, R. A. Guyer, and M. D. Miller, Phys. Rev. B **27**, 474 (1983); R. M. de Leonardis and S. E. Trullinger, *ibid.* **27**, 1867 (1983).

[10]S. de Lillo and P. Sodano, Nuovo Cimento **37**, 380 (1983); O. Hudak, J. Phys. B **16**, 2641 (1983); **16**, 2659 (1983); O. Hudak and L. Trlifaj, J. Phys. A **18**, 445 (1985).

[11](a) C. R. Willis, M. El-Batanouny, S. Burdick, R. Boesch, and P. Sodano, Phys. Rev. B **35**, 3486 (1987); (b) R. Boesch, P. Stancioff, and C. R. Willis, *ibid.* **38**, 6713 (1988).

[12]R. Giachetti, P. Sodano, E. Sorace, and V. Tognetti, Phys. Rev. B **30**, 4014 (1984).

[13]H. J. Mikeska, J. Phys. C **13**, 2913 (1980).

[14]R. Pandit and C. Tanneous, Phys. Rev. B **28**, 281 (1983); R. Pandit, C. Tanneous, and J. A. Krumhansl, *ibid.* **28**, 289 (1983).

[15]R. Dingle, M. E. Lines, and S. L. Holt, Phys. Rev. **187**, 648 (1969).

[16]J. A. Holyst and A. Sukiennicki, J. Phys. C **18**, 2411 (1985); Phys. Rev. B **28**, 4062 (1983).

[17]T. Munakata, J. Phys. Soc. Jpn. **52**, 1635 (1983); S. Iwabuchi, Prog. Theor. Phys. **70**, 941 (1983).

[18]U. Harten, J. P. Toennies, and Ch. Wöll, Phys. Rev. Lett. **54**, 621 (1985); M. El-Batanouny, S. Burdick, K. M. Martini, and P. Stancioff, *ibid.* **58**, 611 (1987).

[19]R. Rajaraman and M. Rajlakshmi, Phys. Rev. B **25**, 1866 (1982).

[20]P. Sodano, M. El-Batanouny, and C. R. Willis, Phys. Rev. B **34**, 4936 (1986).

[21]S. S. Burdick, M. El-Batanouny, and C. R. Willis, Phys. Rev. B **34**, 6575 (1986); S. Burdick, C. R. Willis, and M. El-Batanouny, *ibid.* **36**, 6920 (1987).

[22]K. Sasaki, Prog. Theory Phys. **70**, 593 (1983); Phys. Rev. B **33**, 7743 (1986).

[23]P. Stancioff, Ph.D. thesis, Boston University, 1988.

[24]H. Segur, J. Math. Phys. **24**, 1439 (1983); M. Rice, Phys. Rev. B **28**, 3587 (1983).

[25]S. Flugge, *Practical Quantum Mechanics* (Springer-Verlag, Berlin, 1874).

[26]R. G. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, Berlin, 1982).