Analytic statistical mechanics for a two-component-kink system

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We employ the transfer-integral technique to study the classical statistical mechanics of a two-component field governed by the Montonen-Sarker-Trullinger-Bishop (MSTB) Hamiltonian. The two-dimensional pseudo-Schrödinger equation approximation to the transfer-integral eigenvalue problem is separated into two one-dimensional Schrödinger equations by transforming to a coordinate system in which the two-component kink trajectories are constant-coordinate lines. This separation of variables allows us to obtain analytic expressions for the low-temperature free energy and static correlation length and we identify contributions to these quantities from the known topological kink excitations in the MSTB model. In addition, we find an unexpected activated contribution to the free energy which we interpret as due to an unknown nontopological kink excitation whose energy vanishes at the bifurcation point.

I. INTRODUCTION

The subject of statistical mechanics of quasi-one-dimensional kink-bearing systems[1] has proved to be a remarkably active area of condensed matter physics in the last few years, beginning with the work of Krumhansl and Schrieffer[2] (KS) and Aubry[3] on the "ϕ-four" model. The ideal-kink-gas phenomenology proposed by KS as a realistic and powerful framework for statistical mechanics calculations at low temperatures has subsequently been shown by Currie, Krumhansl, Bishop, and Trullinger[4] (CKBT) to be *exact* (in the limit of low temperatures) if one properly takes into account the influence of kinks on the phonon density of states.[5] CKBT demonstrated this remarkable "asymptotic exactness" of the phenomenology for kink-bearing, one-component (scalar) fields of the nonlinear Klein-Gordon variety[1,4] (e.g., ϕ-four, sine Gordon, etc.) by explicitly comparing phenomenological results with those obtainable using the exact (and independent) transfer-operator method.[6,7] An explicit comparison was possible because *analytic* forms of the lowest few transfer-operator eigenvalues could be obtained via a modified WKB method[8] for "tunnel-splitting"[2] contributions *and* analytic solutions for the kinks and their associated phonons[9–13] were available for the particular systems considered [ϕ-four, sine-Gordon (SG), and double-quadratic[12,13] (DQ) local potentials]. (We have shown[14] very recently that the asymptotic exactness of the low-temperature CKBT phenomenology can be demonstrated quite generally without explicit knowledge of the kink waveform or its small oscillations.) Recent extensions of the CKBT theory have been made to include systems bearing more than one type of kink[15] (e.g., double-sine-Gordon) and also systems with a finite winding-number density.[16]

All of the investigations cited above have dealt exclusively with one-component (scalar) fields. Although these model systems (such as sine-Gordon) can be used to describe a wide variety of nonlinear phenomena in condensed matter,[17] it is probably fair to say that the majority of effort has been focused on one-component fields at least in part because of the relative ease with which necessary calculations can be carried quite far analytically. However, one-component-field models by no means span the entire range of interesting phenomena. On the contrary, an equally wide variety[17] of nonlinear condensed-matter systems require, by their very nature, a description based on multicomponent fields. Perhaps the most extreme example of current interest is superfluid ^{3}He, which is in principle described[18] by a tensor field with 9 complex components or *18* real fields. (Fortunately, only two or three independent combinations of these fields are needed in practice.) Less formidable (but no less interesting) examples include charge-density-wave condensates,[19–22] Ginzburg-Landau theory for superconductors,[23,24] Heisenberg spin systems,[25] and the XY model,[26,27] to mention a few.

When compared to the CKBT theory[4] for one-component-kink systems, the corresponding theory for the general class of *two*-component (complex scalar) kink-bearing nonlinear fields in one dimension is still in its infancy. There are two basic reasons for its stunted growth: (i) the dearth of analytic solitary-wave solutions to relevant coupled equations of motion and (ii) the difficulty in developing a general method for obtaining analytic expressions for the lowest eigenvalue(s) of the appropriate transfer operator which is sophisticated enough to isolate the "tunneling" contribution[2,4] that is expected to arise from kink activation. Nevertheless, the success of CKBT theory for one-component kinks gives cause to

be optimistic in applying the *lessons*[1] learned in developing that phenomenology to more complicated and realistic situations. The primary lesson is that kinks having a finite (nonzero) threshold creation energy will form a dilute gas at low temperatures and that the gas can be regarded as "ideal" if the sharing of degrees of freedom among kinks and phonons is accounted for in the phenomenology.

We wish to emphasize, therefore, that we have no *a priori* reason to doubt the validity of an ideal-gas phenomenology for multicomponent kinks in one dimension. Nevertheless, it would be most comforting if at least *one* nontrivial example of a multicomponent–kink-bearing system could be found for which the statistical mechanics can be *analytically* investigated at low temperatures.

In this paper, we elaborate the discovery by one of us[28] that there is indeed such a very simple model, far from trivial, which is susceptible to analytic progress. In this model, a dimensionless complex scalar field

$$\psi(x,t) = |\psi(x,t)| \exp[i\phi(x,t)] \ ,$$

is governed by the Lagrangian density[29–32]

$$\mathcal{L} = \tfrac{1}{2}|\psi_t|^2 - \tfrac{1}{2}|\psi_x|^2 - V(|\psi|,\phi) \ , \tag{1.1}$$

where the subscripts x and t denote derivatives with respect to the dimensionless space (x) and time (t) coordinates, respectively, and $V(|\psi|,\phi)$ is a dimensionless "local potential" having the form

$$V(|\psi|,\phi) = \tfrac{1}{4}(1-|\psi|^2)^2 + \tfrac{1}{4}\kappa|\psi|^2\sin^2\phi \ . \tag{1.2}$$

Here κ is a dimensionless positive constant governing the degree of "phase anisotropy" possessed by the potential. The first term in Eq. (1.2) represents a "rotated ϕ-four" potential[2–4] having the shape of the "bottom of a wine bottle." The second term breaks the continuous rotational symmetry by introducing indentations in the wine-bottle potential so that two degenerate minima are formed at $\psi = \pm 1$. Plots of this potential and its equipotential contours for several values of κ can be found in Ref. 31. In addition to providing perhaps the simplest two-component generalization of the one-component models considered by CKBT,[4] this model also has the very attractive feature that the single-kink solitary wave solutions to the coupled nonlinear equations of motion [obtained from Eq. (1.1)] have been found analytically by Sarker, Trullinger, and Bishop[29] (STB) (and independently by Montonen[30]), and we shall hereafter refer to this model as the MSTB model. Interestingly, an additional "nontopological" kink solution has recently been obtained by Rajaraman[32] (for the special case $\kappa = \frac{1}{4}$), about which we shall comment in detail below in Sec. V.

The equations of motion following from Eq. (1.1) take very simple forms in terms of the real (ξ) and imaginary (η) parts of the complex field $\psi = \xi + i\eta$:

$$\xi_{tt} - \xi_{xx} - \xi + \xi(\xi^2+\eta^2) = 0 \ , \tag{1.3a}$$

$$\eta_{tt} - \eta_{xx} - (1-\tfrac{1}{2}\kappa)\eta + \eta(\xi^2+\eta^2) = 0 \ . \tag{1.3b}$$

The analytic single-kink solutions fall into two classes.[29–31] The class-one solutions are purely real:

$$\xi_1^{\pm}(s) = \pm\tanh(s/\sqrt{2}) \ , \tag{1.4a}$$

$$\eta_1^{\pm}(s) = 0 \ , \tag{1.4b}$$

where $s \equiv \gamma(x-vt)$ is the "rest frame" variable [$\gamma = (1-v^2)^{-1/2}$], and $\pm$ denotes a kink (+) or antikink (−). The class-two solutions have two homotopic varieties (labeled by 2 and 2*) and exist only for $\kappa < 1$:

$$\xi_2^{\pm}(s) = \pm\tanh(\sqrt{\kappa/2}s) \ , \tag{1.5a}$$

$$\eta_2^{\pm}(s) = (1-\kappa)^{1/2}\,\mathrm{sech}(\sqrt{\kappa/2}s) \ , \tag{1.5b}$$

and

$$\xi_{2^*}^{\pm}(s) = \pm\tanh(\sqrt{\kappa/2}s) \ , \tag{1.6a}$$

$$\eta_{2^*}^{\pm}(s) = -(1-\kappa)^{1/2}\,\mathrm{sech}(\sqrt{\kappa/2}s) \ , \tag{1.6b}$$

where again the $\pm$ signs denote kinks (+) and antikinks (−). The trajectories (in the $\xi-\eta$ plane) followed by these various kinks as they evolve the field from one minimum in V to another are shown schematically in Fig. 1. The class-one solutions are independent of κ and are the only single-kink solutions found for $\kappa \geq 1$. The class-two solutions exist only for $\kappa < 1$ and degenerate to class-one solutions at $\kappa = 1$. The energies of the traveling kink solutions

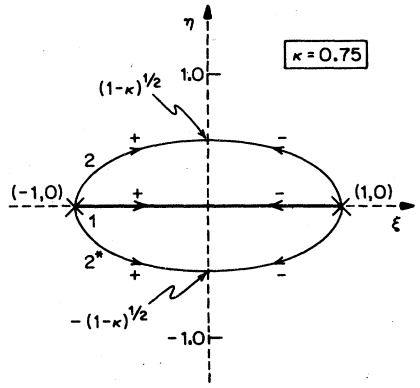

FIG. 1. Topological kink trajectories in the MSTB model. For $\kappa > 1$, only the class-one kink (+) and antikink (−) exist while for $\kappa < 1$, the class-one kinks become unstable and are replaced by the class-two kinks which follow semielliptical paths between the two potential minima (indicated by crosses).

are[29]

$$E_1(v) = \gamma E_1(0) = \gamma \tfrac{2}{3}\sqrt{2} \ , \tag{1.7a}$$

and

$$E_2(v) = E_{2^*}(v) = \gamma E_2(0) = \gamma\sqrt{2\kappa}(1 - \tfrac{1}{3}\kappa) \ . \tag{1.7b}$$

When $\kappa = 1$ the rest energies of the two classes of kinks are equal and for $\kappa < 1$, $E_2(0) < E_1(0)$. This suggests that a class-one kink is unstable to decay into a class-two kink satisfying the same boundary conditions when $\kappa < 1$. Indeed, linear stability analysis[29,33] shows that class-one kinks are stable for all κ against fluctuations in ξ but are unstable to growth in η for $\kappa < 1$. The class-two kinks are stable for $\kappa < 1$ against fluctuations in both ξ and η. The parameter point $\kappa = 1$ is thus regarded[29] as a "bifurcation point" in the sense that as κ is decreased past unity, a second type of solution appears while the first becomes unstable. STB[29] pointed out the fact that the class-one kinks are just the familiar ϕ-four kinks while in the limit $\kappa \to 0^+$ the stable class-two kinks approach those of the familiar sine-Gordon theory ($|\psi|$ is nearly constant in this limit). Thus the complex-scalar MSTB theory exhibits a very interesting "crossover" behavior between the two well-studied real scalar field theories.

The classical statistical mechanics of the MSTB Hamiltonian [corresponding to Eqs. (1.1) and (1.2)] has been studied previously by Currie, Sarker, Bishop, and Trullinger[31] (CSBT) using a "brute-force" *numerical* evaluation of the lowest few eigensolutions of the effective "Schrödinger equation approximation" to the transfer-integral equation[1-4,6-8] in the continuum limit (kink width >> lattice constant) (see Sec. II below). Using an ansatz for the temperature dependence of the "tunneling" free energy,[2] CSBT were led to conclude that the low-temperature static correlation length for the field grows exponentially with decreasing temperature, at a rate determined by the activation energy for the solitary wave (kink) appropriate to the κ value of interest. The activation energy was obtained by fitting the *assumed* form to the actual numerical values of the lowest eigenvalues, and was in agreement with Eq. (1.7) for the kink rest energies. In particular, the crossover behavior as κ (denoted by 8D/A in Ref. 31) varies through the bifurcation point ($\kappa = 1$) was dramatically demonstrated (Fig. 9 of Ref. 31). As we shall see, however, the exponential form assumed for the "tunnel splitting" (difference of the lowest two eigenvalues) by CSBT was not quite correct[34]; it had the wrong power of temperature in the prefactor of the exponential. In addition, by focusing on the *difference* of the two lowest eigenvalues, CSBT did not notice another exponential contribution to these eigenvalues which cancels when the difference is taken. However, the free energy, being the lowest eigenvalue of the transfer operator, contains this extra contribution. This suggests the existence of another type of excitation heretofore unknown and not even suspected. Our analytic results therefore demonstrate quite dramatically the danger of assuming that the ideal-gas phenomenology can be trivially carried over to two-component problems.

We begin our detailed discussion in Sec. II with a brief exposition of the transfer-operator method as applied to our two-component model Hamiltonian, arriving at the effective Schrödinger equation approximation[6] to the transfer integral equation in the continuum limit. In this two-dimensional problem, the fields ξ and η play the role of "coordinates" and thus the calculation of statistical mechanical quantities is reduced to the problem of solving for the "energy eigenvalues" and "eigenfunctions" for a pseudoquantum "particle" moving in the two-dimensional potential $V(\xi, \eta)$. In Sec. III we motivate our transformation from the "Cartesian" coordinates (ξ, η) to elliptic polar coordinates[35] (u, v). The kink trajectories in Fig. 1 become constant-coordinate lines in this new coordinate system and we find that the two-dimensional Schrödinger equation of Sec. II *separates* into two one-dimensional equations which are solved analytically at low temperatures in Sec. IV to obtain the lowest two eigenvalues, which in turn give the low-temperature free energy and static correlation length for the MSTB model. In addition to containing contributions from the kinks described above, the free energy also contains an unexpected contribution which we attempt to interpret in Sec. V as due to an additional type of elementary excitation. Although the precise form of this predicted solution to Eqs. (1.3) is not yet known, we shall extract a great deal of information about its qualitative nature from the statistical mechanics results, together with simple arguments involving the energetics of known solutions. Finally, in Sec. VI we summarize our results and discuss their implications for other two-component models and for the development of ideal-gas phenomenologies.

II. TRANSFER-OPERATOR METHOD AND THE "SCHRÖDINGER EQUATION" APPROXIMATION

In this section we briefly review the transfer-operator method as it applies to the calculation of the classical canonical partition and static correlation functions for our two-component problem. The symmetry properties of the transfer operator are discussed since they have direct bearing on the nature of its eigenfunctions and will be used in the subsequent discussion. In the continuum limit the transfer-integral equation is replaced by its "Schrödinger-equation" representation. The solution

of this Schrödinger problem forms the basis for discussion in the following sections.

In discretized form the Hamiltonian corresponding to Eq. (1.1) is given by

$$H = l \sum_{i=1}^{N} \left[\tfrac{1}{2} |\dot{\psi}_i|^2 + \frac{1}{2l^2} |\psi_{i+1} - \psi_i|^2 + V(|\psi_i|, \phi_i) \right] , \tag{2.1}$$

where l is a dimensionless discretization length (e.g., lattice constant), N is the number of "sites" along the "chain" of length $L = Nl$, a dot denotes a time derivative, and $V(|\psi_i|, \phi_i)$ is the dimensionless, local (on-site) potential whose form will be kept general until we later specialize to the particular case of interest, namely Eq. (1.2). Thus, the discussion in this section applies also to the case of the fourfold anisotropic potential discussed recently by Subbaswamy and Trullinger,[36] for example. In terms of the real and imaginary parts of ψ, we can write

$$H = l \sum_{i=1}^{N} \left[\tfrac{1}{2} (\dot{\xi}_i^2 + \dot{\eta}_i^2) + \frac{1}{2l^2} (\xi_{i+1} - \xi_i)^2 + \frac{1}{2l^2} (\eta_{i+1} - \eta_i)^2 + V(\xi_i, \eta_i) \right] , \tag{2.2}$$

where the MSTB potential of interest is

$$V(\xi_i, \eta_i) = \tfrac{1}{4} [1 - (\xi_i^2 + \eta_i^2)]^2 + \tfrac{1}{4} \kappa \eta_i^2 . \tag{2.3}$$

The canonical partition function can be written in factored form as

$$Z = Z_{\dot{\xi}} Z_{\dot{\eta}} Z_{\xi,\eta} , \tag{2.4}$$

where the kinetic contributions, $Z_{\dot{\xi}}$ and $Z_{\dot{\eta}}$, are given by

$$Z_{\dot{\xi}} = Z_{\dot{\eta}} = \prod_{i=1}^{N} \frac{1}{h} \int_{-\infty}^{+\infty} d\dot{\xi}_i \, e^{-\beta l \dot{\xi}_i^2/2} = \left(\frac{2\pi l}{\beta h^2} \right)^{N/2} \tag{2.5}$$

$$[\beta = (k_B T)^{-1}] .$$

Here, Planck's constant is understood to be expressed in the characteristic units of the system. The configurational contribution to the partition function is given by

$$Z_{\xi,\eta} = \prod_{i=1}^{N} \int_{-\infty}^{+\infty} d\xi_i \int_{-\infty}^{+\infty} d\eta_i \exp\left[-\beta l \left(\frac{1}{2l^2} (\xi_{i+1} - \xi_i)^2 + \frac{1}{2l^2} (\eta_{i+1} - \eta_i)^2 + V(\xi_i, \eta_i) \right) \right] . \tag{2.6}$$

As for the one-component problems considered by CKBT,[4] we impose periodic boundary conditions $[(\xi_{N+1}, \eta_{N+1}) = (\xi_1, \eta_1)]$ and introduce δ functions to enforce these conditions:

$$Z_{\xi,\eta} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\xi_{N+1} \, d\eta_{N+1} \cdots \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\xi_1 \, d\eta_1 \, \delta(\xi_{N+1} - \xi_1) \delta(\eta_{N+1} - \eta_1) \times \exp[-\beta l f(\xi_{N+1}, \eta_{N+1}; \xi_N, \eta_N)] \times \cdots \times \exp[-\beta l f(\xi_2, \eta_2; \xi_1, \eta_1)] , \tag{2.7}$$

where $f(\xi_{i+1}, \eta_{i+1}; \xi_i, \eta_i)$ is defined by

$$f(\xi_{i+1}, \eta_{i+1}; \xi_i, \eta_i) \equiv \frac{1}{2l^2} (\xi_{i+1} - \xi_i)^2 + \frac{1}{2l^2} (\eta_{i+1} - \eta_i)^2 + \tfrac{1}{2} [V(\xi_i, \eta_i) + V(\xi_{i+1}, \eta_{i+1})] . \tag{2.8}$$

Note that we have taken advantage of the δ functions to make $f(\xi_{i+1}, \eta_{i+1}; \xi_i, \eta_i)$ symmetric under the interchange $(\xi_i, \eta_i) \leftrightarrow (\xi_{i+1}, \eta_{i+1})$.

We now expand the δ function product

$$\delta(\xi_{N+1} - \xi_1) \delta(\eta_{N+1} - \eta_1)$$

in terms of a complete set of orthonormal functions $\{\Phi_n(\xi, \eta)\}$:

$$\delta(\xi_{N+1} - \xi_1) \delta(\eta_{N+1} - \eta_1) = \sum_n \Phi_n^*(\xi_{N+1}, \eta_{N+1}) \Phi_n(\xi_1, \eta_1) . \tag{2.9}$$

We conveniently choose the functions $\{\Phi_n(\xi, \eta)\}$ to be eigenfunctions of the two-dimensional transfer integral operator $\hat{T}$, defined by

$$\hat{T}\Phi(\xi_i, \eta_i) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\xi_i \, d\eta_i \times \exp[-\beta l f(\xi_{i+1}, \eta_{i+1}; \xi_i, \eta_i)] \times \Phi(\xi_i, \eta_i) , \tag{2.10}$$

so that

$$\hat{T}\Phi_n(\xi_i, \eta_i) = e^{-\beta l \epsilon_n} \Phi_n(\xi_{i+1}, \eta_{i+1}) , \tag{2.11}$$

where ϵ_n is the eigenvalue associated with $\Phi_n(\xi, \eta)$. With this choice, it is easy to see that $Z_{\xi,\eta}$ becomes

$$Z_{\xi,\eta} = \sum_n e^{-\beta L \epsilon_n} . \tag{2.12}$$

In the thermodynamic limit ($L \to \infty$), the free energy density $f = F/L = -(k_B T/L) \ln Z$ is given simply

by

$$f=-(\beta l)^{-1}\ln\left[\frac{2\pi l}{\beta h^2}\right]+\epsilon_0 \ , \tag{2.13}$$

where ϵ_0 is the lowest eigenvalue of $\hat{T}$. The other thermodynamic functions (internal energy, specific heat, etc.) can be obtained using their standard relations to f.

The average of some function $g(\xi,\eta)$ is given by

$$\langle g(\xi,\eta)\rangle=\int_{-\infty}^{+\infty}d\xi\int_{-\infty}^{+\infty}d\eta\,\mathcal{P}(\xi,\eta)g(\xi,\eta) \ , \tag{2.14}$$

where the probability distribution function $\mathcal{P}(\xi,\eta)$, is the squared modulus of the "ground state" eigenfunction $\Phi_0(\xi,\eta)$ of $\hat{T}$:

$$\mathcal{P}(\xi,\eta)=|\Phi_0(\xi,\eta)|^2 \ . \tag{2.15}$$

General expressions for equal time correlation functions can be found straightforwardly

$$\langle g_1(\xi_i,\eta_i)g_2(\xi_j,\eta_j)\rangle = \sum_n \langle 0|g_1(\xi,\eta)|n\rangle\langle n|g_2(\xi,\eta)|0\rangle \times\exp[-\beta(\epsilon_n-\epsilon_0)l|i-j|] \ , \tag{2.16a}$$

and

$$\langle \delta g_1(\xi_i,\eta_i)\delta g_2(\xi_j,\eta_j)\rangle = \sum_{n\neq 0} \langle 0|g_1(\xi,\eta)|n\rangle\langle n|g_2(\xi,\eta)|0\rangle \times\exp[-\beta(\epsilon_n-\epsilon_0)l|i-j|] \ , \tag{2.16b}$$

where

$$\delta g(\xi,\eta)\equiv g(\xi,\eta)-\langle g(\xi,\eta)\rangle$$

and we have used bra-ket notation to denote overlap matrix elements

$$\langle m|g(\xi,\eta)|n\rangle \equiv\int_{-\infty}^{+\infty}d\xi\int_{-\infty}^{+\infty}d\eta\,\Phi_m^*(\xi,\eta)g(\xi,\eta)\Phi_n(\xi,\eta) \ . \tag{2.17}$$

In order to determine which adjoint states $\langle n|$ are coupled to the ground state $|0\rangle$ by a function $g(\xi,\eta)$, it is helpful to have "selection rules" at hand. For the particular case of the MSTB potential Eq. (2.3), $V(\xi,\eta)$ has C_{2v} point group symmetry[37] in the ξ and η variables. As a consequence it is not difficult to show that the transfer integral operator $\hat{T}$, commutes with all operations in the point group C_{2v}, i.e.,

$$[\hat{T},\hat{P}_R]=0 \ , \tag{2.18}$$

where $\hat{P}_R$ is the function operator representative of a proper or improper two-dimensional rotation R in C_{2v}. Denoting the "coordinate" pair (ξ,η) as a two-dimensional vector $\vec{r}=\xi\hat{\xi}+\eta\hat{\eta}$, and by $\vec{\mathrm{R}}$ a 2×2 orthogonal matrix representative of R, we have[37]

$$\hat{P}_R g(\vec{r})\equiv g(\vec{\mathrm{R}}^{-1}\vec{r}) \ . \tag{2.19}$$

Setting $\vec{r}=\vec{r}_i$ in Eq. (2.19) and acting from the left with $\hat{T}$, we have

$$\hat{T}\hat{P}_R g(\vec{r}_i)=\int\int d^2\vec{r}_i\exp[-\beta l f(\vec{r}_{i+1};\vec{r}_i)] \times g(\vec{\mathrm{R}}^{-1}\vec{r}_i) \ . \tag{2.20}$$

Since $\vec{\mathrm{R}}$ is an orthogonal "rotation," we can replace $\vec{r}_i$ everywhere in the integrand in Eq. (2.20) by $\vec{\mathrm{R}}\,\vec{r}_i$ without affecting the value of the integral (since it extends over the entire two space). Thus,

$$\hat{T}\hat{P}_R g(\vec{r}_i)=\int\int d^2\vec{r}_i\exp[-\beta l f(\vec{r}_{i+1};\vec{\mathrm{R}}\vec{r}_i)]g(\vec{r}_i) \ . \tag{2.21}$$

Now, we again make use of the orthogonality of $\vec{\mathrm{R}}$ (a rotation leaves scalar products invariant) and the invariance of $V(\vec{r})$ to write

$$\begin{aligned} f(\vec{r}_{i+1};\vec{\mathrm{R}}\vec{r}_i) &= \frac{1}{2l^2}(\vec{r}_{i+1}-\vec{\mathrm{R}}\vec{r}_i)\cdot(\vec{r}_{i+1}-\vec{\mathrm{R}}\vec{r}_i)+\tfrac{1}{2}[V(\vec{\mathrm{R}}\vec{r}_i)+V(\vec{r}_{i+1})] \\ &= \frac{1}{2l^2}[\vec{\mathrm{R}}^{-1}(\vec{r}_{i+1}-\vec{\mathrm{R}}\vec{r}_i)]\cdot[\vec{\mathrm{R}}^{-1}(\vec{r}_{i+1}-\vec{\mathrm{R}}\vec{r}_i)]+\tfrac{1}{2}[V(\vec{r}_i)+V(\vec{r}_{i+1})] \\ &= \frac{1}{2l^2}(\vec{\mathrm{R}}^{-1}\vec{r}_{i+1}-\vec{r}_i)\cdot(\vec{\mathrm{R}}^{-1}\vec{r}_{i+1}-\vec{r}_i)+\tfrac{1}{2}[V(\vec{r}_i)+V(\vec{\mathrm{R}}^{-1}\vec{r}_{i+1})] \\ &= f(\vec{\mathrm{R}}^{-1}\vec{r}_{i+1};\vec{r}_i) \ . \end{aligned} \tag{2.22}$$

Thus,

$$\hat{T}\hat{P}_R g(\vec{r}_i)=\int\int d^2\vec{r}_i\exp[-\beta l f(\vec{\mathrm{R}}^{-1}\vec{r}_{i+1};\vec{r}_i)]g(\vec{r}_i)=\hat{P}_R\int\int d^2\vec{r}_i\exp[-\beta l f(\vec{r}_{i+1};\vec{r}_i)]g(\vec{r}_i)=\hat{P}_R\hat{T}g(\vec{r}_i) \tag{2.23}$$

and Eq. (2.18) is proved.

Since the transfer integral operator commutes with the operations in the point group C_{2v}, then the eigenfunctions of $\hat{T}$ must also serve as basis functions for the irreducible representations of C_{2v}. The standard techniques of group theory[37] may therefore be used to "block diagonalize" $\hat{T}$, or to obtain the "selection rules" mentioned above for matrix elements. Further discussion of this latter topic will be postponed until Sec. IV where we discuss correlation functions at low temperatures. We shall, however, make use of the basis function requirement in Sec. III in order to determine the transformation properties of the eigenfunctions in a different (and more convenient) coordinate system.

The technique for converting the transfer integral operator to a differential operator having Schrödinger form in the continuum limit ($l \to 0$) has been outlined previously by Scalapino, Sears, and Ferrell.[6] Here we give a discussion, parallel to theirs, which accounts for the completeness requirement on the eigenfunctions $\{\Phi_n(\xi,\eta)\}$. The effects of lattice discreteness ($l \neq 0$) may then be taken into account[38] (or at least estimated) by retaining higher order terms in l. Although we shall not explicitly examine discrete-lattice corrections in this paper, we feel it is important to set the stage for such an investigation, since in applications to physical systems we must consider the importance of lattice discreteness.

In order to convert the two-dimensional Fredholm integral equation represented by Eqs. (2.10) and (2.11) to a differential form in the limit $l \ll 1$, we proceed as follows. First we define an auxiliary function,

$$\Psi_n(\xi,\eta) \equiv e^{-\beta l V(\xi,\eta)/2}\Phi_n(\xi,\eta) \ , \tag{2.24}$$

so that Eq. (2.11) may be rewritten with the use of Eq. (2.8) as

$$\int_{-\infty}^{+\infty} d\xi_i \int_{-\infty}^{+\infty} d\eta_i \exp\left[-\beta l\left(\frac{1}{2l^2}(\xi_{i+1}-\xi_i)^2+\frac{1}{2l^2}(\eta_{i+1}-\eta_i)^2\right)\right]\Psi_n(\xi_i,\eta_i)$$
$$= \exp\{-\beta l[\epsilon_n - V(\xi_{i+1},\eta_{i+1})]\}\Psi_n(\xi_{i+1},\eta_{i+1}) \ . \tag{2.25}$$

In the limit $l \ll 1$, the integrations over ξ_i and η_i are dominated by those values close to ξ_{i+1} and η_{i+1}, respectively. By expanding $\Psi_n(\xi_i,\eta_i)$ about $\Psi_n(\xi_{i+1},\eta_{i+1})$ in a double Taylor series, Eq. (2.25) can be rewritten in differential form as (dropping the $i+1$ subscript)

$$\exp\left\{l(m^*)^{1/2}\left[\frac{1}{2m^*}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)\right]\right\}\Psi_n(\xi,\eta)$$
$$= \exp\{-l(m^*)^{1/2}[\epsilon_n - V_0 - V(\xi,\eta)]\}\Psi_n(\xi,\eta) \ , \tag{2.26}$$

where m^* and V_0 are defined by

$$m^* \equiv \beta^2 \ , \tag{2.27}$$

$$V_0 \equiv [(m^*)^{1/2}l]^{-1}\ln\left(\frac{(m^*)^{1/2}}{2\pi l}\right) \ . \tag{2.28}$$

Using Eq. (2.24), we can rearrange Eq. (2.26) to yield an equation for the original eigenfunction $\Phi_n(\xi,\eta)$:

$$\exp[-\tfrac{1}{2}l(m^*)^{1/2}V(\xi,\eta)]\exp\left[l(m^*)^{1/2}\left[\frac{1}{2m^*}\nabla^2\right]\right]$$
$$\times\exp[-\tfrac{1}{2}l(m^*)^{1/2}V(\xi,\eta)]\Phi_n(\xi,\eta)$$
$$= \exp[-l(m^*)^{1/2}(\epsilon_n - V_0)]\Phi_n(\xi,\eta) \ , \tag{2.29}$$

where $\nabla^2 \equiv \partial^2/\partial\xi^2 + \partial^2/\partial\eta^2$.

Up to this point we have made no approximation and Eq. (2.29) is entirely equivalent to the transfer integral Eqs. (2.10) and (2.11). When $l \ll 1$, we may make use of the identity

$$e^B e^A e^B = \exp\left\{A + 2B + \frac{1}{3!}[A+B,[A,B]] + \cdots\right\} \ , \tag{2.30}$$

which is valid through fourth order in A and B, to rewrite Eq. (2.29) in the approximate form

$$\left\{-\frac{\nabla^2}{2m^*} + V(\xi,\eta)\right.$$
$$\left. + \tfrac{1}{24}l^2\left[\frac{\nabla^2}{m^*} - V(\xi,\eta),[\nabla^2,V(\xi,\eta)]\right] + O(l^4)\right\}$$
$$\times\Phi_n(\xi,\eta) = (\epsilon_n - V_0)\Phi_n(\xi,\eta) \ . \tag{2.31}$$

To lowest order in l^2, we are thus faced with a pseudo-Schrödinger equation,

$$\left(-\frac{1}{2m^*}\nabla^2 + V(\xi,\eta)\right)\Phi_n(\xi,\eta)$$
$$= (\epsilon_n - V_0)\Phi_n(\xi,\eta) \ , \tag{2.32}$$

for a single "particle" of "mass" m^* moving in the two-dimensional, anisotropic potential $V(\xi,\eta)$. We note that V_0 acts as a temperature-dependent "energy" minimum which is important for the free energy,

entropy, etc., but not for the correlation lengths which depend only on eigenvalue differences [see Eq. (2.16)]. No real quantum mechanics is involved ($\hbar$ is replaced[6] essentially by the temperature, i.e., $m^* \sim T^{-2}$) but intuition and techniques from quantum mechanics can be very helpful. For example, the influence of the lattice-discreteness term ($\sim l^2$) in Eq. (2.31) can be obtained via first-order perturbation theory. The change induced in the eigenvalue ϵ_n is thus found to be

$$\Delta\epsilon_n = -\tfrac{1}{12} l^2 \int_{-\infty}^{+\infty} d\xi \int_{-\infty}^{+\infty} d\eta \left[\left(\frac{\partial V}{\partial \xi} \right)^2 + \left(\frac{\partial V}{\partial \eta} \right)^2 \right] \times |\Phi_n(\xi,\eta)|^2 \ , \quad (2.33)$$

where $\Phi_n(\xi,\eta)$ is a normalized solution of the unperturbed equation (2.32). The use of Eq. (2.33) allows one to obtain[38] discrete-lattice corrections to the thermodynamic functions and correlation lengths.

III. TRANSFORMATION TO KINK-PATH COORDINATES AND THE SEPARATION OF VARIABLES

In this section we begin our discussion of the analytic solution of the effective Schrödinger equation (2.32) for the lowest eigenvalues relevant to the thermodynamic functions. We motivate and carry out a transformation to a coordinate system in which the two-dimensional Schrödinger equation can be reduced to two *one*-dimensional Schrödinger equations via the method of separation of variables. We also give a detailed discussion of the symmetry properties of the eigenfunctions in this new coordinate system, since these properties prove to be very useful in carrying out the solution of the separated equations at low temperatures as described in Sec. IV.

We begin by rewriting Eq. (2.32) in a slightly scaled form,

$$\left[-\frac{1}{2\tilde{m}} \left(\frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right) + [1 - (\xi^2+\eta^2)]^2 + \kappa\eta^2 \right] \times \Phi_n(\xi,\eta) = \tilde{\epsilon}_n \Phi_n(\xi,\eta) \ , \quad (3.1)$$

where we have used Eq. (2.3) and the definitions

$$\tilde{m} \equiv \tfrac{1}{4} m^* \quad (3.2)$$

and

$$\tilde{\epsilon}_n \equiv 4(\epsilon_n - V_0) \ . \quad (3.3)$$

As noted in Sec. II, we are faced with the problem of solving a pseudo-Schrödinger equation (3.1) for a "particle" of "mass" $\tilde{m}$ moving in the anisotropic two-dimensional potential $\tilde{V}(\xi,\eta)$:

$$\tilde{V}(\xi,\eta) \equiv [1 - (\xi^2+\eta^2)]^2 + \kappa\eta^2 \ . \quad (3.4)$$

The motivation for making the coordinate transformation described below is based on the recognition that the solution of Eq. (3.1) for the ground-state eigenvalue (i.e., the configurational free energy density [see Eq. (2.13)] should contain a "tunneling" portion corresponding to the MSTB[29,30] kinks at low temperatures ($\tilde{m} \gg 1$), in analogy with the corresponding tunneling contribution from the scalar kinks in the one-component problems discussed by CKBT.[4] Whereas this tunneling portion can be calculated via the WKB method[39] or its improved variants[8,40,41] in the case of the general class of one-component kink systems,[4,7] there appears to be no equally systematic "two-dimensional" WKB method which can be applied to anisotropic two-dimensional potentials such as $\tilde{V}(\xi,\eta)$. However, we note that the kink trajectory followed in $\xi-\eta$ space (see Fig. 1) serves as a very special path from one minimum of the anisotropic potential to another degenerate minimum, and that perhaps the 2D WKB problem reduces to an effective 1D WKB problem(s) by considering the appropriate kink trajectory to be the "tunneling path." This very simple intuitive hunch has indeed proved to be correct, and by transforming to a coordinate system in which the kink trajectory is a constant-coordinate line, we have managed to obtain analytic solutions to Eq. (3.1) at low temperatures (Sec. IV).

From the work of MSTB,[29,30] we know the analytic form of the kink trajectories in $\xi-\eta$ space. As shown schematically in Fig. 1, the kinks follow semi-elliptical paths when $\kappa < 1$ and a straight line path between the two minima when $\kappa > 1$. The elliptical shape of the trajectory prompts us to transform from the "Cartesian" coordinates (ξ,η) to elliptical-polar coordinates[35] u and v:

$$\xi = a \cosh u \cos v \ , \quad (3.5a)$$

$$\eta = a \sinh u \sin v \ , \quad (3.5b)$$

where $0 \leq u < \infty$ and $-\pi \leq v \leq \pi$. Constant values of u describe concentric ellipses while constant values of v describe semihyperbolas normal to these ellipses. These families of curves are shown in Fig. 2. By choosing the constant a in Eqs. (3.5) to be

$$a \equiv \sqrt{\kappa} \ , \quad (3.6)$$

we find that the kink trajectories for *both* $\kappa < 1$ and $\kappa > 1$ are described by constant values of u with v varying between the limits given below:

$$\kappa \leq 1$$

$$u = u_\kappa = \cosh^{-1}(\kappa^{-1/2}), \quad 0 \leq |v| \leq \pi \quad (3.7a)$$

or

$$\kappa \geq 1$$

$$u = u_\kappa = 0 \ , \quad \cos^{-1}(\kappa^{-1/2}) \leq |v| \leq \pi - \cos^{-1}(\kappa^{-1/2}) \ . \quad (3.7b)$$

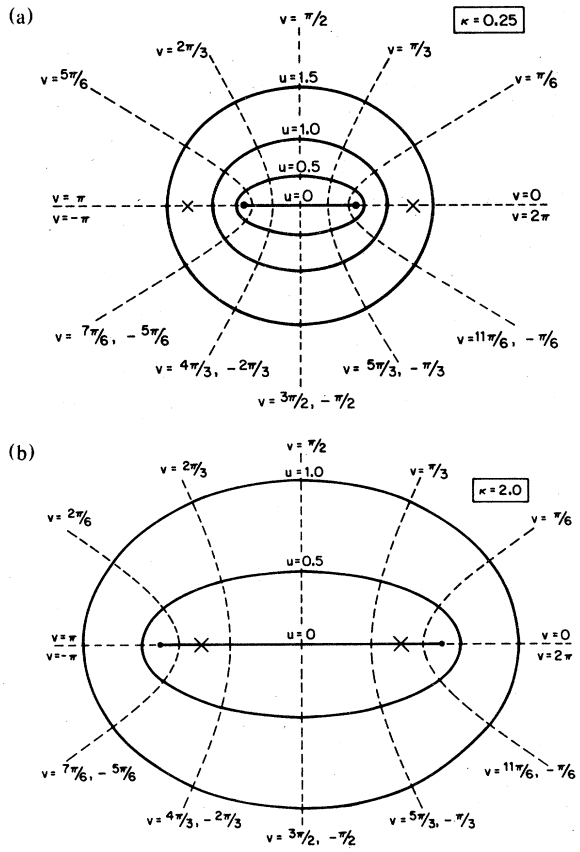

FIG. 2. Constant-coordinate lines in the elliptic-polar coordinate system. Constant values of the elliptic radius (u) describe concentric ellipses with $u=0$ being the degenerate ellipse connecting the two foci (dots) at $(\pm\sqrt{\kappa},0)$. The dashed semihyperbolas are lines of constant elliptic angle (v) normal to the ellipses. For $\kappa<1$ (a), the foci lie inside the potential minima, while for $\kappa>1$ (b), the foci lie outside the minima.

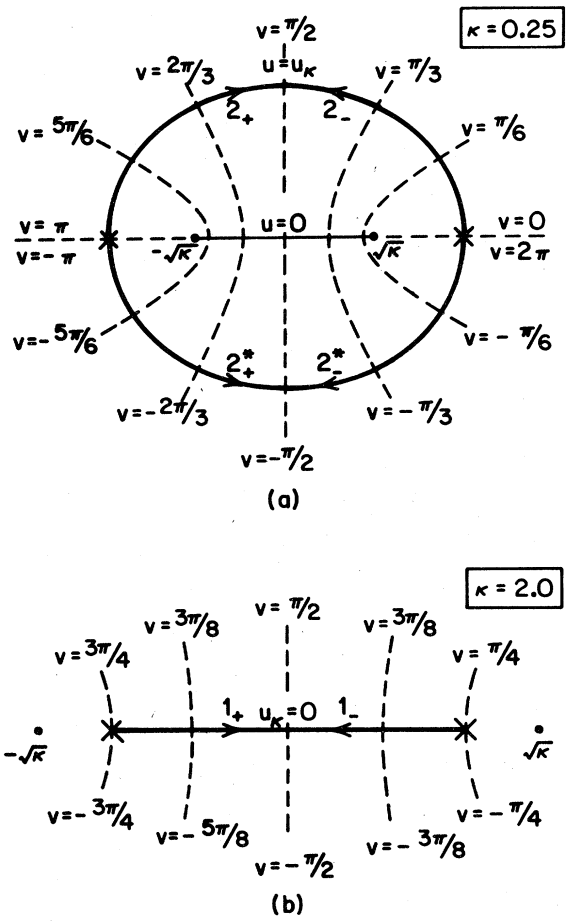

FIG. 3. Topological kink trajectories in the elliptic coordinate system. (a) The class-two kink ($\kappa<1$) follows a semiellipse $[u=u_\kappa=\cosh^{-1}(\kappa^{-1/2})]$ with $|v|$ varying between zero and π. (b) The class-one kink follows the $u=0$ line between $v=\cos^{-1}(\kappa^{-1/2})$ and $\pi-\cos^{-1}(\kappa^{-1/2})$.

Examples of these trajectories in the elliptic coordinate system are shown in Fig. 3.

In terms of the elliptic coordinates (u,v), Eq. (3.1) becomes

$$\tilde{H}\Phi_n(u,v)=\epsilon_n\Phi_n(u,v)\ , \tag{3.8}$$

where

$$\tilde{H}=-\frac{1}{2\tilde{m}\kappa}(\sinh^2u+\sin^2v)^{-1}\left[\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\right]$$
$$+(1-\kappa)^2-2\kappa(1-\kappa)(\sinh^2u-\sin^2v)$$
$$+\kappa^2(\sinh^4u-\sinh^2u\sin^2v+\sin^4v)\ . \tag{3.9}$$

When we compare this form of the Hamiltonian to that in Eq. (3.1), it may appear at first glance that we have hopelessly complicated the problem by such a transformation. *However*, let us multiply Eq. (3.8) by the Jacobian factor[35] $(\sinh^2u+\sin^2v)$ and use Eq. (3.9) to obtain

$$-\frac{1}{2\tilde{m}\kappa}\left[\frac{\partial^2\Phi_n}{\partial u^2}+\frac{\partial^2\Phi_n}{\partial v^2}\right]+(1-\kappa)^2(\sinh^2u+\sin^2v)\Phi_n$$
$$-2\kappa(1-\kappa)(\sinh^4u-\sin^4v)\Phi_n$$
$$+\kappa^2(\sinh^6u+\sin^6v)\Phi_n=\tilde{\epsilon}_n(\sinh^2u+\sin^2v)\Phi_n\ . \tag{3.10}$$

Note that in this form, the effective Schrödinger equation contains *no mixed terms* in u and v. This implies that Eq. (3.10) is separable. Indeed, if we as-

sume a factored form for $\Phi(u,v)$,

$$\Phi(u,v)=R(u)\chi(v) \ , \tag{3.11}$$

then Eq. (3.10) can be written as

$$-\frac{1}{2\tilde{m}\kappa}\frac{R''(u)}{R(u)}+(1-\kappa\cosh^2u)^2\sinh^2u-\tilde{\epsilon}\sinh^2u$$
$$=\frac{1}{2\tilde{m}\kappa}\frac{\chi''(v)}{\chi(v)}-(1-\kappa\cos^2v)^2\sin^2v+\tilde{\epsilon}\sin^2v$$
$$\equiv\Delta \ , \tag{3.12}$$

where Δ is a separation constant which must be independent of both u and v.

The primary consequence of this separation is, of course, that we now only need to deal with one-dimensional equations (although two of them) instead of the original two-dimensional Schrödinger equation (3.1), i.e., Eq. (3.12) may be rewritten as two equations which both have the one-dimensional Schrödinger form:

$$-\frac{1}{2\tilde{m}\kappa}\frac{d^2R(u)}{du^2}$$
$$+[(1-\kappa\cosh^2u)^2\sinh^2u-\tilde{\epsilon}\sinh^2u]R(u)$$
$$=\tilde{\epsilon}_uR(u) \tag{3.13a}$$

and

$$-\frac{1}{2\tilde{m}\kappa}\frac{d^2\chi(v)}{dv^2}$$
$$+[(1-\kappa\cos^2v)^2\sin^2v-\tilde{\epsilon}\sin^2v]\chi(v)$$
$$=\tilde{\epsilon}_v\chi(v) \ , \tag{3.13b}$$

where, according to Eq. (3.12) we must require that

$$\tilde{\epsilon}_u=\Delta=-\tilde{\epsilon}_v \ . \tag{3.14}$$

Note that in these two Schrödinger equations, the eigenvalues determine the allowed values of the separation constant Δ, while the original eigenvalue $\tilde{\epsilon}$ now appears as part of the "potential" function in each equation. Thus, Eqs. (3.13) and (3.14) must be solved in a self-consistent fashion. In other words, the eigenvalues of the original equation (3.1) are the values of $\tilde{\epsilon}$ for which the eigenspectra sets $\{\tilde{\epsilon}_u\}$ and $\{-\tilde{\epsilon}_v\}$ have at least one element in common.

In the next section, we show how to carry out such a self-consistent procedure for the lowest few eigenvalues at low temperatures, with particular regard to isolating the "tunneling" contributions to $\tilde{\epsilon}_0$. For that purpose it is helpful to have a knowledge of the symmetry properties of the eigenfunctions $\{\Phi(u,v)=R(u)\chi(v)\}$ in the elliptical-polar coordinate system and we devote the remainder of this section to a discussion of these properties.

In Sec. II we proved that the operations in the point group C_{2v} commute with the transfer integral operator and as a consequence the eigenfunctions $\Phi_n(\xi,\eta)$ must provide basis functions for the irreducible representations of C_{2v}. The same is true, of course, for the Schrödinger approximation Eq. (3.1) for these eigenfunctions, and furthermore, it must also be the case that the product eigenfunctions $\Phi_n(u,v)=R_n(u)\chi_n(v)$ must serve as basis functions in the elliptical-polar coordinate system introduced above. The one-dimensional "potentials,"

$$U_1(u)\equiv(1-\kappa\cosh^2u)^2\sinh^2u-\tilde{\epsilon}\sinh^2u \ , \tag{3.15a}$$

$$V_1(v)\equiv(1-\kappa\cos^2v)^2\sin^2v-\tilde{\epsilon}\sin^2v \ , \tag{3.15b}$$

which appear in the separated equations (3.13a) and (3.13b), respectively, reflect the C_{2v} symmetry possessed by the original two-dimensional potential $\tilde{V}(\xi,\eta)$ [Eq. (3.4)]. Thus, the one-dimensional eigenfunctions $R(u)$ and $\chi(v)$ can be classified according to their transformation properties under the operations in C_{2v}, which can be formally carried out in either of the two ways shown in Table I. The "radial" functions $R(u)$ have either even or odd parity and the "angular" functions $\chi(v)$ are either π or 2π periodic, with even or odd parity. The appropriate combinations satisfying the basis function requirement are shown in Table I, along with the character table for C_{2v}.

In the elliptical-polar coordinate system the normalization condition on the eigenfunctions reads as

$$\kappa\int_0^\infty du\int_{-\pi}^{\pi}dv\,(\sinh^2u+\sin^2v)|\Phi_n(u,v)|^2$$
$$=\kappa\int_0^\infty du\,\sinh^2u|R_n(u)|^2\int_{-\pi}^{\pi}dv\,|\chi_n(v)|^2$$
$$+\kappa\int_0^\infty du\,|R_n(u)|^2\int_{-\pi}^{\pi}dv\,\sin^2v|\chi_n(v)|^2$$
$$=1 \ . \tag{3.16}$$

Matrix elements such as Eq. (2.17) take the form

$$\langle m|g(u,v)|n\rangle$$
$$=\kappa\int_0^\infty du\int_{-\pi}^{\pi}dv\,(\sinh^2u+\sin^2v)$$
$$\times\Phi_m^*(u,v)g(u,v)\Phi_n(u,v) \ . \tag{3.17}$$

Selection rules for these matrix elements can be obtained by noting that the Jacobian, $J=\kappa(\sinh^2u+\sin^2v)$, is invariant under C_{2v} and therefore the product

$$\Phi_m^*(u,v)g(u,v)\Phi_n(u,v)$$

must contain a portion[37] which transforms as the

TABLE I. Character table for the irreducible representations of C_{2v}. Also shown are two ways of formally carrying out the symmetry operations in the elliptic-polar (u, v) coordinate system. The parities and periodicities of the eigenfunctions [Eq. (3.11)] serving as basis functions are indicated by the subscripts.

Basis functions	Rep.	$u \to u$, $v \to v$ / $u \to u$, $v \to v$ E	$u \to u$, $v \to v+\pi$ / $u \to -u$, $v \to \pi - v$ C_2	$u \to u$, $v \to -v$ / $u \to -u$, $v \to v$ σ_ξ	$u \to u$, $v \to \pi - v$ / $u \to u$, $v \to \pi - v$ σ_η
$R_+(u)\chi_{\pi,+}(v)$	A_1	1	1	1	1
$R_-(u)\chi_{\pi,-}(v)$	A_2	1	1	−1	−1
$R_+(u)\chi_{2\pi,+}(v)$	B_1	1	−1	1	−1
$R_-(u)\chi_{2\pi,-}(v)$	B_2	1	−1	−1	1

identity representation (A_1 in Table I) in order for the matrix element Eq. (3.17) to be nonzero. Of particular interest in the next section will be the correlation function for the fluctuations in the field:

$$C_{\delta\psi^*,\delta\psi}(|i-j|) \equiv \langle \delta\psi_i^* \delta\psi_j \rangle \ . \tag{3.18}$$

Since

$$\psi[=\xi+i\eta=\sqrt{\kappa}(\cosh u\cos v + i\sinh u \sin v)]$$

contains only portions of $B_1(\xi)$ and $B_2(\eta)$ symmetry (see Table I), then the only states coupled to the ground state (A_1 symmetry) must have either B_1 or B_2 symmetry. In the limit of large separation, $|i-j| \to \infty$, it is the lowest "excited" state coupled to the ground state which dominates the sum over states in Eq. (2.16b). For the correlation function Eq. (3.18) this is the first excited state, which happens to have B_1 symmetry, and $C_{\delta\psi^*,\delta\psi}$ becomes

$$C_{\delta\psi^*,\delta\psi} \underset{|i-j|\to\infty}{\to} \kappa^2 \left| \int_0^\infty du \int_{-\pi}^{+\pi} dv\, (\sinh^2 u + \sin^2 v)\cosh u \cos v \Phi_1^*(u,v)\Phi_0(u,v) \right|^2 e^{-|i-j|l/\lambda} \tag{3.19}$$

where the correlation length λ is given by

$$\lambda = [\beta(\epsilon_1 - \epsilon_0)]^{-1} \ . \tag{3.20}$$

In the next section we obtain analytic expressions for ϵ_0 and ϵ_1 at low temperatures and hence the free energy and correlation length.

IV. LOW-TEMPERATURE FREE ENERGY AND FIELD CORRELATION LENGTH

In this section we describe our method for solving Eqs. (3.13) and (3.14) self-consistently and present the resulting low-temperature analytic expressions for the lowest two eigenvalues, $\tilde{\epsilon}_0$ and $\tilde{\epsilon}_1$, which in turn give the configurational free energy density [Eq. (2.13)] and the correlation length λ, for field fluctuations at equal times [Eqs. (3.19) and (3.20)].

We recall from Eq. (2.13) that the free energy density f, has two contributions

$$f = f_{\dot{\psi}} + f_\psi \ , \tag{4.1}$$

where $f_{\dot{\psi}}$ is the "kinetic" part,

$$f_{\dot{\psi}} = -(\beta l)^{-1} \ln\left(\frac{2\pi l}{\beta h^2}\right) \ , \tag{4.2}$$

and f_ψ is the "configurational" or "potential" part,

$$f_\psi = \epsilon_0 = \tfrac{1}{4}\tilde{\epsilon}_0 + V_0 \ , \tag{4.3}$$

where V_0 is given in Eq. (2.28) and $\tilde{\epsilon}_0$ is the lowest eigenvalue of Eq. (3.1). To obtain $\tilde{\epsilon}_0$ at low temperatures, we first note that, by analogy with the one-component problems discussed by CKBT,[4] we expect $\tilde{\epsilon}_0$ to be equal to the ground state of an isolated well minus an exponentially small "tunnel splitting." The first excited state $\tilde{\epsilon}_1$ is then the tunnel-split partner to $\tilde{\epsilon}_0$. The ground state of an isolated well may be obtained easily from Eq. (3.1) by considering the anisotropic 2D harmonic oscillator potential which approximates $[1-(\xi^2+\eta^2)]+\kappa\eta^2$ near $(\xi,\eta)=(\pm 1, 0)$. We then find that this ground-state harmonic oscillator eigenvalue is given by

$$\tilde{\epsilon}_0^{(0)} = (\sqrt{2}+\sqrt{\kappa/2})\tilde{m}^{-1/2} \ . \tag{4.4}$$

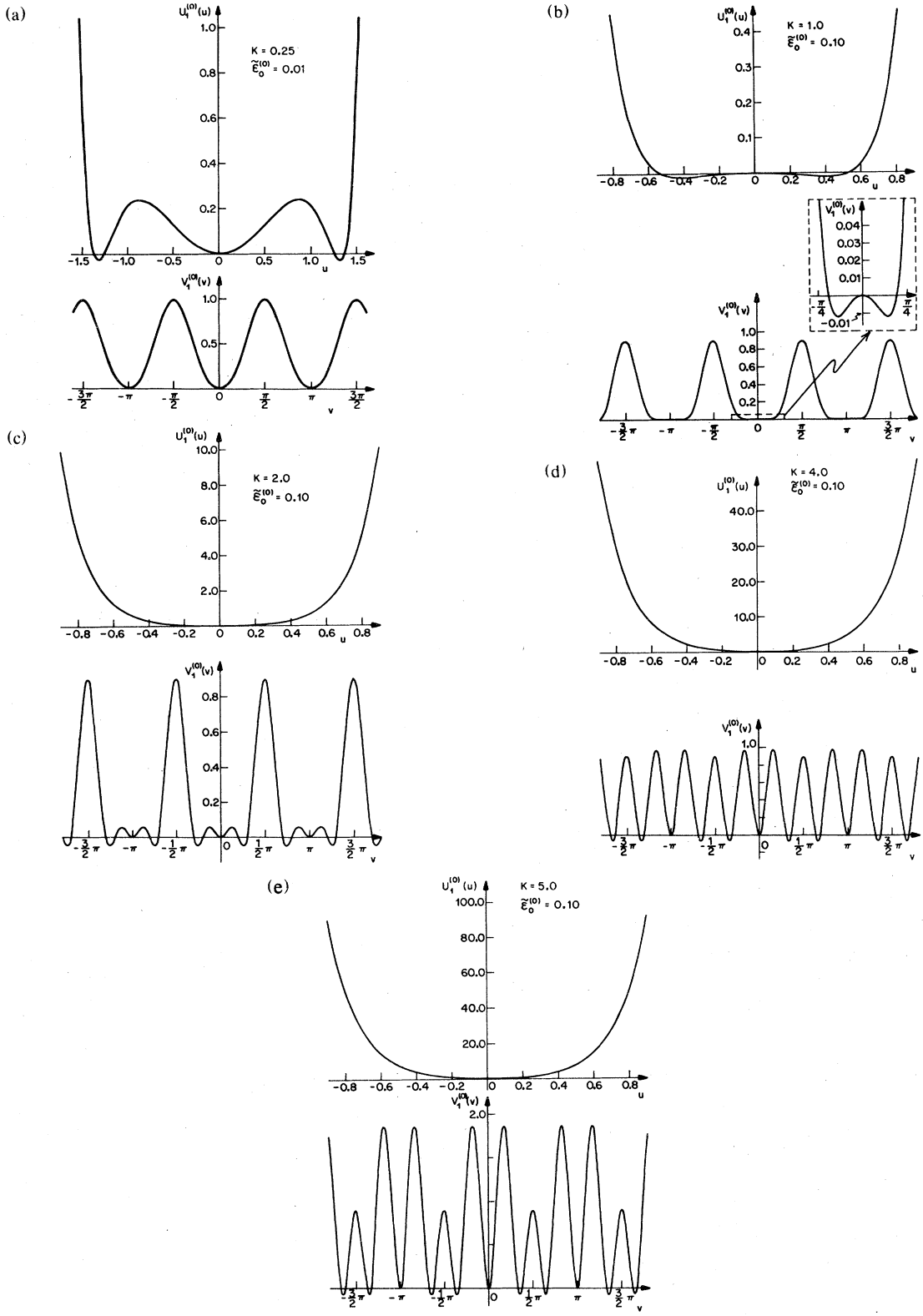

FIG. 4. One-dimensional potentials appearing in the separated Schrödinger equations (4.7) for various values of the anisotropy parameter, κ: (a) 0.25, (b) 1.0, (c) 2.0, (d) 4.0, and (e) 5.0. Note the different scales used and also the choice of $\tilde{\epsilon}_0^{(0)} = 0.01$ for (a) and $\tilde{\epsilon}_0^{(0)} = 0.10$ for (b)–(e).

We thus expect $\tilde{\epsilon}_0$ to have the low-temperature form

$$\tilde{\epsilon}_0 = \tilde{\epsilon}_0^{(0)} - t_0 \tag{4.5}$$

and

$$\tilde{\epsilon}_1 = \tilde{\epsilon}_0^{(0)} + t_1 \ , \tag{4.6}$$

where t_0 and t_1 are exponentially small tunneling contributions which remain to be calculated.

The way in which t_0 is found proceeds as follows. We first find the ground state eigenvalues, $\tilde{\epsilon}_{u,0}^{(0)}$ and $\tilde{\epsilon}_{v,0}^{(0)}$, of Eqs. (3.13a) and (3.13b), respectively, when $\tilde{\epsilon}$ is set equal to $\tilde{\epsilon}_0^{(0)}$, i.e., when t_0 is neglected. We then regard the inclusion of the exponentially small t_0 as a perturbation and calculate the resulting shift in $\tilde{\epsilon}_{u,0}$ and $\tilde{\epsilon}_{v,0}$ via first-order perturbation theory. The actual value of t_0 is then obtained by setting $\tilde{\epsilon}_{u,0} = -\tilde{\epsilon}_{v,0}$ according to Eq. (3.14).

The "unperturbed" ($t_0 = 0$) Schrödinger equations are

$$-\frac{1}{2\tilde{m}\kappa}\frac{d^2R^{(0)}(u)}{du^2} + U_1^{(0)}(u)R^{(0)}(u) = \tilde{\epsilon}_u^{(0)}R^{(0)}(u) \tag{4.7a}$$

and

$$-\frac{1}{2\tilde{m}\kappa}\frac{d^2\chi^{(0)}(v)}{dv^2} + V_1^{(0)}(v)\chi^{(0)}(v) = \tilde{\epsilon}_v^{(0)}\chi^{(0)}(v) \ , \tag{4.7b}$$

where the one-dimensional "unperturbed" potential functions $U_1^{(0)}$ and $V_1^{(0)}$ are obtained from Eqs. (3.15) setting $\tilde{\epsilon} = \tilde{\epsilon}_0^{(0)}$. In Fig. 4 we have plotted these potentials for the example cases $\kappa = \frac{1}{4}$, 1, 2, 4, 5. In these plots we have arbitrarily chosen $\tilde{\epsilon}_0^{(0)}$ for illustration. (In the limit as $T \to 0$, $\tilde{\epsilon}_0^{(0)} \to 0$.) Note that although we shall normalize the radial functions over positive u values only, we have plotted $U_1^{(0)}(u)$ for negative u as well since its formal symmetry yields even and odd solutions, and both types are necessary for proper symmetry of the eigenfunctions (Table I). Similarly, we have plotted $V_1^{(0)}(v)$ for a range larger than the fundamental period $-\pi \leq v \leq \pi$ since the formal periodicity of V_1 will also prove to be useful in obtaining $\tilde{\epsilon}_{v,0}^{(0)}$, by exploiting the analogy to energy band problems.

Once the unperturbed ground state eigenvalues $\{\tilde{\epsilon}_{u,0}^{(0)}, \tilde{\epsilon}_{v,0}^{(0)}\}$ and their corresponding eigenfunctions $\{R_0^{(0)}(u), \chi_0^{(0)}(v)\}$ have been determined from Eqs. (4.7) we can treat the perturbations due to t_0. In doing so it is necessary to exercise some care in the normalization conventions. We let

$$R_0^{(0)}(u) = N_u \bar{R}_0^{(0)}(u) \ , \tag{4.8a}$$

where

$$\int_0^\infty du\, |\bar{R}_0^{(0)}(u)|^2 = 1 \ , \tag{4.8b}$$

and, similarly,

$$\chi_0^{(0)}(v) = N_v \bar{\chi}_0^{(0)}(v) \ , \tag{4.9a}$$

$$\int_{-\pi}^{\pi} dv\, |\bar{\chi}_0^{(0)}(v)|^2 = 1 \ . \tag{4.9b}$$

The overall normalization condition Eq. (3.16) then requires that the product $N_u N_v$ satisfy

$$N_0 \equiv N_u^2 N_v^2 = \frac{1}{\kappa}\left[\int_0^\infty du\, \sinh^2 u\, |\bar{R}_0^{(0)}(u)|^2 + \int_{-\pi}^{\pi} dv\, \sin^2 v\, |\bar{\chi}_0^{(0)}(v)|^2\right]^{-1} \ . \tag{4.10}$$

The inclusion of the perturbing potentials

$$U_1^{(1)}(u) = t_0 \sinh^2 u \tag{4.11a}$$

and

$$V_1^{(1)}(v) = t_0 \sin^2 v \ , \tag{4.11b}$$

can be carried out using standard first-order bound-state perturbation theory. The full ground-state eigenvalues $\tilde{\epsilon}_{u,0}$ and $\tilde{\epsilon}_{v,0}$ are given to first order in t_0 by

$$\tilde{\epsilon}_{u,0} = \tilde{\epsilon}_{u,0}^{(0)} + t_0 \int_0^\infty du\, \sinh^2 u\, |\bar{R}_0^{(0)}(u)|^2 \tag{4.12a}$$

and

$$\tilde{\epsilon}_{v,0} = \tilde{\epsilon}_{v,0}^{(0)} + t_0 \int_{-\pi}^{\pi} dv\, \sin^2 v\, |\bar{\chi}_0^{(0)}(v)|^2 \ . \tag{4.12b}$$

Substitution of Eqs. (4.12) into Eq. (3.14) finally yields an expression for t_0

$$t_0 = -\kappa N_0(\tilde{\epsilon}_{u,0}^{(0)} + \tilde{\epsilon}_{v,0}^{(0)}) \tag{4.13a}$$

and, in a similar fashion

$$t_1 = +\kappa N_0(\tilde{\epsilon}_{u,0}^{(0)} + \tilde{\epsilon}_{v,1}^{(0)}) \ , \tag{4.13b}$$

where we have used Eq. (4.10). As we shall see, the eigenvalues in brackets in Eqs. (4.13) combine to give exponentially small factors, so that t_0 and t_1 are exponentially small at low temperatures, as expected. Note that we have used $\tilde{\epsilon}_{u,0}^{(0)}$ in Eq. (4.13b) for t_1 as well as t_0. This is because the lowest two states of the full potential have the *same* radial eigenfunction $[R_{0,+}(u)]$ factor, which is symmetric in u, i.e., the lowest two states have A_1 and B_1 symmetry, respectively.

We now evaluate t_0 and t_1 for the two cases $\kappa < 1$ and $\kappa > 1$. The special case $\kappa = 1$ (the bifurcation point) will be discussed afterwards.

A. $\kappa < 1$

In this case, the unperturbed one-dimensional potentials $U_1^{(0)}(u)$ and $V_1^{(0)}(v)$ have the general shape

shown in Fig. 4(a) where plots are given for $\kappa=\frac{1}{4}$ with $\tilde{\epsilon}_0^{(0)}$ arbitrarily set to 0.01 for illustration. From the formal periodicity of $V_1^{(0)}(v)$, the eigenfunctions $\chi^{(0)}(v)$ in principle have Bloch form, with eigenvalues forming a band structure. However, since we include only π and 2π periodic functions in our complete set, we need only the states at the band extrema ["Brillouin zone" center (π periodic) and zone edge (2π periodic)]. At low temperatures, where $\tilde{m}\gg 1$, the two lowest eigenvalues $\tilde{\epsilon}_{v,0}^{(0)}$ and $\tilde{\epsilon}_{v,1}^{(0)}$, can be written as

$$\tilde{\epsilon}_{v,0}^{(0)}=\tilde{\epsilon}_{v,0}^{(0)H}-t_v \tag{4.14a}$$

and

$$\tilde{\epsilon}_{v,1}^{(0)}=\tilde{\epsilon}_{v,0}^{(0)H}+t_v \ , \tag{4.14b}$$

where $\epsilon_{v,0}^{(0)H}$ is the harmonic ground state ("zero-point energy") of a single well of $V_1^{(0)}(v)$ and t_v is the half-width of the lowest band of eigenvalues. The corresponding ground-state wave function $\chi_0^{(0)}(v)$ is π periodic, has even parity, and is sharply peaked about each well of $V_1^{(0)}(v)$. The second state $\chi_1^{(0)}(v)$ is 2π periodic, even, and also sharply peaked about the wells. To obtain $\tilde{\epsilon}_{v,0}^{(0)H}$ we expand $V_1^{(0)}(v)$ to second order in v about $v=0$:

$$V_1^{(0)}(v)\cong[(1-\kappa)^2-\tilde{\epsilon}_0^{(0)}]v^2 \ . \tag{4.15}$$

Substitution of Eq. (4.15) into Eq. (4.7b) and retention of only the leading power of the small quantity $\tilde{m}^{-1/2}$ yields [using Eq. (4.4)]

$$\tilde{\epsilon}_{v,0}^{(0)H}\cong\frac{1-\kappa}{\sqrt{2\kappa}}\tilde{m}^{-1/2} \ . \tag{4.16}$$

The ground state radial function $R_0^{(0)}(u)$ is symmetric in u and sharply peaked about the minima of $U_1^{(0)}(u)$. These are located approximately at

$$u_0\cong\pm\sinh^{-1}\left[\frac{1-\kappa}{\kappa}+\frac{\tilde{\epsilon}_0^{(0)}}{2\kappa(1-\kappa)}\right]^{1/2}$$
$$\underset{\tilde{m}\to\infty}{\to}\pm\sinh^{-1}\left[\frac{1-\kappa}{\kappa}\right]^{1/2}=\pm u_\kappa \ , \tag{4.17}$$

where u_κ [Eq. (3.7a)] is the value of u for the kink trajectory. From the shape of $U_1^{(0)}(u)$ we expect $\tilde{\epsilon}_{u,0}^{(0)}$ to be the ground state of an isolated well minus a tunnel-splitting t_u

$$\tilde{\epsilon}_{u,0}^{(0)}=\tilde{\epsilon}_{u,0}^{(0)H}-t_u \ . \tag{4.18}$$

Near $u=u_0$, $U_1^{(0)}(u)$ is approximately given by

$$U_1^{(0)}(u)\cong-\frac{(1-\kappa)}{\kappa}\tilde{\epsilon}_0^{(0)}+\frac{4(1-\kappa)^2}{\kappa}(u-u_0)^2 \ . \tag{4.19}$$

By making use of Eqs. (4.4), (4.7a), and (4.19), we thus find

$$\tilde{\epsilon}_{u,0}^{(0)H}\cong-\frac{1-\kappa}{\sqrt{2\kappa}}\tilde{m}^{-1/2} \ . \tag{4.20}$$

Comparing this result to that obtained for $\tilde{\epsilon}_{v,0}^{(0)H}$ [Eq. (4.16)], we see that these harmonic levels are negatives

$$\tilde{\epsilon}_{u,0}^{(0)H}=-\tilde{\epsilon}_{v,0}^{(0)H} \ . \tag{4.21}$$

Thus,

$$\tilde{\epsilon}_{u,0}^{(0)}+\tilde{\epsilon}_{v,0}^{(0)}=-(t_u+t_v) \ , \tag{4.22}$$

and Eq. (4.13a) for t_0 can be rewritten (for $\kappa<1$) as

$$t_0=\kappa N_0(t_u+t_v) \quad (\kappa<1) \ . \tag{4.23a}$$

Similarly, Eq. (4.13b) becomes

$$t_1=\kappa N_0(-t_u+t_v) \quad (\kappa<1) \ . \tag{4.23b}$$

For the purpose of calculating N_0 according to Eq. (4.10), we can approximate the eigenfunctions by appropriately normalized [Eqs. (4.8b) and (4.9b)] ground-state harmonic oscillator eigenfunctions centered on the well minima. We find that ($\kappa<1$)

$$\int_0^\infty du\,\sinh^2u\,[\bar{R}_0^{(0)}(u)]^2\cong\frac{1-\kappa}{\kappa} \ , \tag{4.24a}$$

and

$$\int_{-\pi}^{\pi}dv\,\sin^2v\,[\bar{\chi}_0^{(0)}(v)]^2$$
$$\cong[2\sqrt{2\kappa}(1-\kappa)]^{-1/2}\tilde{m}^{-1/2} \ . \tag{4.24b}$$

The contribution of the last integral [Eq. (4.24b)] to N_0 is negligible at low temperatures ($\tilde{m}\gg 1$) compared to the contribution of the first [Eq. (4.24a)]. Thus, we have the approximate results

$$t_0\cong\frac{\kappa}{1-\kappa}(t_u+t_v) \ , \tag{4.25a}$$

$$t_1\cong\frac{\kappa}{1-\kappa}(-t_u+t_v) \ . \tag{4.25b}$$

Using the WKB method, we find[41] the following low-temperature expressions for the tunneling contributions t_u and t_v ($\kappa<1$):

$$t_u\cong 4(\pi e)^{-1/2}\kappa^{-5/4}(1-\sqrt{\kappa})\beta^{-1}$$
$$\times\exp[-\beta\sqrt{2}(1-\sqrt{\kappa})^2(2+\sqrt{\kappa})/3] \tag{4.26a}$$

and

$$t_v\cong 8(\pi\sqrt{\kappa/2})^{-1/2}(1+\sqrt{\kappa})^{5/2}(1-\sqrt{\kappa})^{1/2}$$
$$\times\beta^{-1/2}\exp[-\beta\sqrt{2\kappa}(1-\tfrac{1}{3}\kappa)] \ . \tag{4.26b}$$

If we make use of Eqs. (1.7), the arguments of the

exponentials in Eqs. (4.26) can be expressed in terms of the kink rest energies. From Eqs. (4.25), we then have

$$t_0(t_1) \cong \frac{8}{\sqrt{\pi}}\left[\frac{\sqrt{2}\kappa^{3/2}(1+\sqrt{\kappa})^3}{(1-\sqrt{\kappa})}\right]^{1/2}\beta^{-1/2}e^{-\beta E_2^{(0)}} + (-)4(\pi e)^{-1/2}\frac{\kappa^{-1/4}}{(1+\sqrt{\kappa})} \times \beta^{-1}\exp\{-\beta[E_1(0)-E_2(0)]\} \quad (\kappa<1) , \tag{4.27}$$

where $(-)$ is associated with the value of t_1. Note the appearance of the class-two kink rest energy as an activation energy in the first term. This serves as a signature of the class-two kinks in the low-temperature thermodynamics. However, we have an additional contribution which is activated as well, but with the *difference* of the class-one and class-two kink rest energies as an activation energy. We shall have much more to say about this term in a moment. The free energy density is obtained from Eqs. (4.1)–(4.5), (2.28), (3.2), and (4.27):

$$f = f_0 + f_t , \tag{4.28}$$

where

$$f_0 = k_B T\left[\frac{1}{2}(\sqrt{2}+\sqrt{\kappa/2}) + \frac{2}{l}\ln\left[\frac{\beta\hbar}{l}\right]\right] , \tag{4.29}$$

and

$$f_t = -\tfrac{1}{4}t_0 . \tag{4.30}$$

The contribution f_0 is just the classical free energy density expected from small oscillations about the potential well minima ("phonons") and f_t is the "tunneling" free energy density which we can presume from the form Eq. (4.27) to be due to class-two kinks, as expected in CKBT theory,[4] *and* an *unexpected* type of excitation having a minimum activation energy, $E_1(0)-E_2(0)$. The correlation length for equal-time field fluctuations, however, is given by Eq. (3.20)

$$\lambda = [\beta(\epsilon_1-\epsilon_0)]^{-1} = [\tfrac{1}{4}\beta(\tilde{\epsilon}_1-\tilde{\epsilon}_0)]^{-1} = [\tfrac{1}{4}\beta(t_1+t_0)]^{-1} = \tfrac{1}{4}\sqrt{\pi}\left[\frac{\sqrt{2}\kappa^{3/2}(1+\sqrt{\kappa})^3}{(1-\sqrt{\kappa})}\right]^{-1/2}\beta^{-1/2}e^{+\beta E_2^{(0)}} \quad (\kappa<1) , \tag{4.31}$$

and does *not* contain a portion due to the "extra" excitation. We note that the prefactor of the second exponential in Eq. (4.27) may need slight modification due to the fact that unmodified WKB results are known[8] to be incorrect by a factor of $(e/\pi)^{1/2} \cong 0.93$ in the one-component case. We have not yet succeeded in improving these results along the lines discussed in Ref. 8, due to the more complicated structure of the one-dimensional separated potential, $U_1^{(0)}(u)$. Nevertheless, the temperature dependence of t_0 *is* correct; subsequent corrections to t_0 will only arise as numerical temperature-independent factors.

B. $\kappa > 1$

In this case, the unperturbed one-dimensional potentials $U_1^{(0)}(u)$ and $V_1^{(0)}(v)$ have the general shape shown in Figs. 4(c)–4(e) where the plots are given for $\kappa = 2, 4, 5$ with $\tilde{\epsilon}_0^{(0)}$ arbitrarily set to 0.1 for illustration. The radial potential $U_1^{(0)}(u)$ has one minimum at $u = u_\kappa = 0$; there is no radial "tunneling" in this case. At low temperatures ($\tilde{m} >> 1$) the ground-state eigenvalue $\tilde{\epsilon}_{u,0}^{(0)}$ is well approximated by the harmonic value

$$\tilde{\epsilon}_{u,0}^{(0)} = \tilde{\epsilon}_{u,0}^{(0)H} = \frac{\kappa-1}{(2\tilde{m}\kappa)^{1/2}} . \tag{4.32}$$

The angular potential $V_1^{(0)}(v)$ is again π periodic and the formal eigenvalues $\tilde{\epsilon}_{v,0}^{(0)}$ form a band structure, but in contrast to the simple case when $\kappa < 1$, we have a band structure reminiscent of a molecular (or dimerized) one-dimensional crystal. Thus there are *two* bands associated with the harmonic ("atomic") level $\tilde{\epsilon}_{v,0}^{(0)H}$ which arise from "bonding" and "antibonding" "molecular orbitals." Tunneling formulas for a similar potential which arise in the double-sine-Gordon one-component problem have been discussed previously.[14] At low temperatures the ground-state eigenvalue $\tilde{\epsilon}_{v,0}^{(0)}$ can be written as

$$\tilde{\epsilon}_{v,0}^{(0)} = \tilde{\epsilon}_{v,0}^{(0)H} - t_v , \tag{4.33}$$

where t_v is the tunneling contribution and $\tilde{\epsilon}_{v,0}^{(0)H}$ is the harmonic ground state of a single well of $V_1^{(0)}(v)$ centered at $v^{(0)}$, given by

$$\sin^2 v^{(0)} \cong 1 - \frac{1}{\kappa} + \frac{\tilde{\epsilon}_0^{(0)}}{2\kappa(\kappa-1)} ; \tag{4.34}$$

we find

$$\tilde{\epsilon}_{v,0}^{(0)H} \cong -\frac{\kappa-1}{(2\tilde{m}\kappa)^{1/2}} = -\tilde{\epsilon}_{u,0}^{(0)H} . \tag{4.35}$$

Thus, as in the $\kappa < 1$ case, the harmonic levels $\tilde{\epsilon}_{v,0}^{(0)H}$ and $\tilde{\epsilon}_{u,0}^{(0)H}$ are negatives of each other and therefore cancel when $\tilde{\epsilon}_{u,0}^{(0)}$ and $\tilde{\epsilon}_{v,0}^{(0)}$ are substituted into Eq. (4.13) for t_0, i.e.,

$$t_0 = \kappa N_0 t_v \quad (\kappa > 1) . \tag{4.36}$$

There are two contributions to t_v which may be

thought of qualitatively as the splitting of the "bonding" and "antibonding" states referred to above and the half-width of the bonding band. The former arises via "tunneling" through the small barrier between minima in $V_1^{(0)}(v)$ and the latter via "tunneling" through the larger barrier. As can be seen in Figs. 4(c)–4(e), the relative size of the barriers inverts as κ is increased past $\kappa \cong 4$. Denoting the tunneling through the double-peaked barriers centered at $n\pi$ by t_v^{I} and the tunneling through the barriers centered at $\frac{1}{2}(2n+1)\pi$ by t_v^{II}, we write

$$t_v = t_v^{\mathrm{I}} + t_v^{\mathrm{II}} \ . \tag{4.37}$$

Again employing the WKB method, we find low-temperature expressions for t_v^{I} and t_v^{II}:

$$t_v^{\mathrm{I}} \cong 4(\pi e)^{-1/2}\kappa^{-5/4}(\sqrt{\kappa}-1)\beta^{-1} \times \exp[-\beta\sqrt{2}(\sqrt{\kappa}-1)^2(\sqrt{\kappa}+2)/3] \tag{4.38a}$$

and

$$t_v^{\mathrm{II}} \cong 16(\sqrt{2}\pi)^{-1/2}\kappa^{-1}(\sqrt{\kappa}-1)^{1/2}(\sqrt{\kappa}+1)^{3/2}\beta^{-1/2} \times \exp(-\beta 2\sqrt{2}/3) \ . \tag{4.38b}$$

The first excited state (B_1 symmetry) eigenvalue can be written in the form Eq. (4.6) where

$$t_1 = \kappa N_0 (t_v^{\mathrm{II}} - t_v^{\mathrm{I}}) \ . \tag{4.39}$$

Using Eq. (1.7a) and the result

$$N_0 \cong (\kappa-1)^{-1} \quad (\kappa > 1) \ , \tag{4.40}$$

we can write

$$t_0(t_1) \cong 16(\sqrt{2}\pi)^{-1/2}\left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1}\right)^{1/2}\beta^{-1/2}e^{-\beta E_1^{(0)}} + (-)4(\pi e)^{-1/2}\kappa^{-1/4}(\sqrt{\kappa}+1)^{-1}\beta^{-1}e^{-\beta E_X} \quad (\kappa > 1) \ , \tag{4.41}$$

where $(-)$ is associated with the value of t_1, and E_X is defined by

$$E_X \equiv \frac{\sqrt{2}}{3}(\sqrt{\kappa}-1)^2(\sqrt{\kappa}+2) \ . \tag{4.42}$$

Note once again the appearance of the stable kink rest energy [this time $E_1(0)$] as an activation energy in the first term of Eq. (4.41). Again we have an extra contribution which is also activated, but now with an activation energy E_X which *cannot* be rewritten as $E_1(0)-E_2(0)$, as before for $\kappa < 1$, since the class-two kink does not exist for $\kappa > 1$. Nevertheless, we note the curious fact that if the definition Eq. (4.42) of E_X is simply extended below $\kappa = 1$, then $E_X = E_1(0) - E_2(0)$ [see Eq. (4.26a)] for $\kappa < 1$. Thus the same formula Eq. (4.42) for the activation energy of the extra contribution can be used both above and below the bifurcation point. As for $\kappa < 1$, the free energy density at low temperatures is given for $\kappa > 1$ by Eqs. (4.28)–(4.30) and (4.41). The prefactor of the extra exponential contribution to t_0 matches precisely with that for $\kappa < 1$ [see Eq. (4.27)]. Thus, we can write a general expression for the extra contribution to the tunneling free energy valid above and below (but not too close to) $\kappa = 1$:

$$f_{t,X} = -\tfrac{1}{4}t_{0,X} \cong -(\pi e)^{-1/2}\kappa^{-1/4}(\sqrt{\kappa}+1)^{-1}\beta^{-1}e^{-\beta E_X} \ , \tag{4.43}$$

where E_X is given by Eq. (4.42).

The correlation length does not contain the E_X contribution and is given, as in Eq. (4.31), by

$$\lambda = \frac{\sqrt{\pi}}{8}2^{1/4}\left(\frac{\sqrt{\kappa}-1)}{\sqrt{\kappa}+1}\right)^{1/2}\beta^{-1/2}e^{+\beta E_1^{(0)}} \quad (\kappa > 1) \ . \tag{4.44}$$

The contribution of the unknown excitation (energy E_X) to the free energy density relative to that by the known kinks varies as a function of κ. For $\kappa \ll 1$ the $E_X[=E_1(0)-E_2(0)]$ contribution is small compared to that of the class-two kinks. For κ approaching unity, however, the "class X" excitation energy approaches zero [see Eq. (4.42)] and the extra contribution dominates the known kinks both above and below the bifurcation point. The above formulas for the tunnel-splitting contributions therefore cannot be used too close to $\kappa = 1$ since the assumption of t_0 and t_1 being small is not justified. It is thus necessary to treat the bifurcation point $\kappa = 1$ in a special manner. We have not yet succeeded in devising a self-consistent procedure for obtaining analytic expressions for the lowest eigenvalues when $\kappa = 1$. This is due to the fact that the wells in the effective one-dimensional potentials, $U_1^{(0)}(u)$ and $V_1^{(0)}(u)$, are extremely flat [see Fig. 4(b)]. Indeed, if $\tilde{\epsilon}_0^{(0)}$ is ignored, one can see from Eqs. (3.15) that when $\kappa = 1$, the potentials vary as the *sixth* power of the deviation from the well minima, with concommitant problems in developing a reliable tunneling formalism. We hope to address this interesting special case in a future paper. For now, we content ourselves with displaying in Fig. 5 the κ dependence of the tunneling contributions to the configurational free energy due to topological kinks and the unknown nontopological kinks, realizing that the region near $\kappa = 1$ is not accurate.

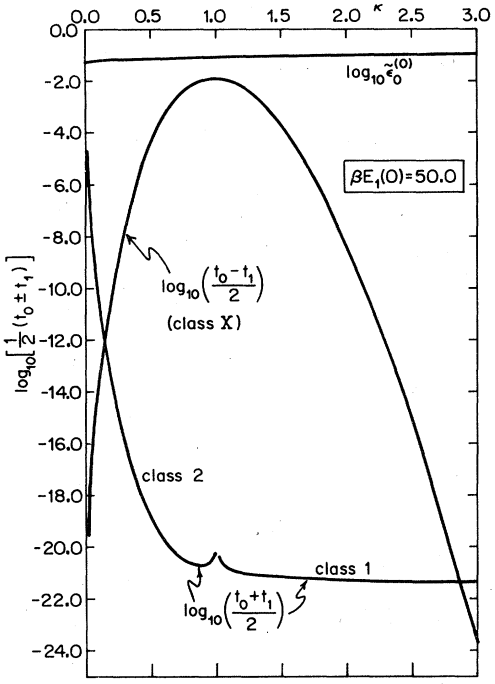

FIG. 5. Kink (tunneling) contributions to the configurational free energy as a function of anisotropy (κ), for $\beta E_1(0)=50.0$. Note the logarithmic vertical scale. The lower curves represent the contribution of the topological kinks while the upper curves represent the contribution of the nontopological "unknown" excitation. The portions of these curves near $\kappa=1$ should not be regarded as accurate since our perturbation theory breaks down near the bifurcation point.

The temperature dependence of the low-temperature correlation length λ, given by Eqs. (4.31) and (4.44) agrees with that obtained for the one-component models studied by CKBT[4] but disagrees with that assumed by CSBT[31] for the prefactor of the exponentials. More detailed numerical studies are currently underway[42] to resolve this discrepancy and to determine the extent of the temperature range over which the analytic results are valid.

In the one-component models,[4] the correlation length for kink-sensitive autocorrelation functions is simply the average spacing between kinks. If $n_K^{\rm tot}$ denotes the total density of kinks plus antikinks, it is thus found in the low-temperature ideal-gas phenomenology that

$$n_k^{\rm tot}=(2\lambda)^{-1} \ . \tag{4.45}$$

Assuming this relationship holds for the present two-component model as well, we can use Eqs. (4.31) and (4.44) to obtain the low-temperature densities of topological kinks:

$$n_{K,1}^{\rm tot}=\frac{1}{d_1}\left[\frac{24}{\pi}\frac{\sqrt{\kappa}+1}{(\sqrt{\kappa}-1)}\right]^{1/2}[\beta E_1(0)]^{1/2}e^{-\beta E_1(0)} \qquad (\kappa>1) \tag{4.46a}$$

and

$$n_{K,2}^{\rm tot}=\frac{\kappa}{d_2}\left[\frac{24}{\pi}\frac{(1+\sqrt{\kappa})^3}{(3-\kappa)(1-\sqrt{\kappa})}\right]^{1/2} \times[\beta E_2(0)]^{1/2}e^{-\beta E_2(0)} \quad (\kappa<1) \ , \tag{4.46b}$$

where we have rewritten the exponential prefactors slightly to enable easy restoration of proper dimensions for lengths and energies. Here d_1 and d_2 are the characteristic widths of the class-one and -two kinks, respectively [in dimensionless units $d_1=\sqrt{2}$ and $d_2=\sqrt{2/\kappa}$; see Eqs. (1.4)–(1.6)].

In the next section we turn our attention to the unknown excitation (energy E_X) and discuss those of its properties which can be deduced from its contribution [Eq. (4.43)] to the configurational free energy and from other energy considerations.

V. UNKNOWN EXCITATION

In this section we try to shed some light on the nature of the excitation which gives rise to the extra term in the tunneling free energy [Eq. (4.43)]. We are in the rare position of having an exact analytic contribution to the low-temperature free energy due to an excitation which was totally unexpected. At this writing, we have not yet been able to find an additional solution to the equations of motion (1.3) which has the activation energy E_X [Eq. (4.42)]. Nevertheless, we can deduce some interesting properties of such a solution from the *form* of its contribution to the free energy together with arguments based on energetics.

First we recall that the unknown excitation does not contribute to the field correlation length λ [see Eqs. (4.31) and (4.44)]. Whereas the class-one and class-two kinks evolve the field between distinct minima in $V(\xi,\eta)$, and thus serve as "change sites" influencing the correlation length, the unknown excitation evidently has the property that the field occupies the *same* minimum of $V(\xi,\eta)$ on both sides of the excitation profile. In other words, if the unknown excitation evolves the field along a trajectory in $\xi-\eta$ space which begins at one of the minima in $V(\xi,\eta)$ and *returns* to the same minimum, then the excitation would not provide a "change site" for the field and as a consequence would not influence the correlation length λ. Thus, we believe that the unknown excitation does indeed follow a trajectory which returns to the originating minimum. Such "nontopological" kink trajectories have been dis-

cussed recently by Rajaraman[32] who has treated a two-component model containing the MSTB model as a subclass. He has found an analytic solution for a nontopological kink for values of his parameters which contain the MSTB case when $\kappa=\frac{1}{4}$. There are two homotopic varieties (which we label 3 and 3*) associated with each minimum in $V(\xi,\eta)$:

$$\xi_3^{\pm}(s)=\pm\left[1-\tfrac{3}{2}\operatorname{sech}^2\left(\frac{s}{2\sqrt{2}}\right)\right], \tag{5.1a}$$

$$\eta_3^{\pm}(s)=\pm\tfrac{3}{2}\operatorname{sech}\left(\frac{s}{2\sqrt{2}}\right)\tanh\left(\frac{s}{2\sqrt{2}}\right), \tag{5.1b}$$

and

$$\xi_{3^*}^{\pm}(s)=\pm\left[1-\tfrac{3}{2}\operatorname{sech}^2\left(\frac{s}{2\sqrt{2}}\right)\right], \tag{5.2a}$$

$$\eta_{3^*}^{\pm}(s)=\mp\tfrac{3}{2}\operatorname{sech}\left(\frac{s}{2\sqrt{2}}\right)\tanh\left(\frac{s}{2\sqrt{2}}\right), \tag{5.2b}$$

where the upper signs refer to kinks associated with the minimum at $(\xi,\eta)=(1,0)$ and the lower signs to kinks associated with the minimum at $(\xi,\eta)=(-1,0)$. Here, $s=\gamma(x-vt)$ is the rest frame coordinate. The various class-three kink trajectories for $\kappa=\frac{1}{4}$ are plotted in Fig. 6. A 3_ kink profile is shown in Fig. 7.

Although the Rajaraman kink solution (class 3) for $\kappa=\frac{1}{4}$ has the required feature that it returns the field to the starting minimum and therefore might be a candidate for the unknown excitation, it unfortunately does *not* have the required activation energy. Whereas we seek a solution with energy $E_X=E_1(0)-E_2(0)$ $(\kappa<1)$, which for $\kappa=\frac{1}{4}$ is

$$E_X=\tfrac{2}{3}\sqrt{2}-\tfrac{11}{24}\sqrt{2}=\tfrac{5}{24}\sqrt{2}\quad(\kappa=\tfrac{1}{4}), \tag{5.3}$$

the Rajaraman kink has rest energy[43]

$$E_3(0)=\tfrac{9}{8}\sqrt{2}\quad(\kappa=\tfrac{1}{4}). \tag{5.4}$$

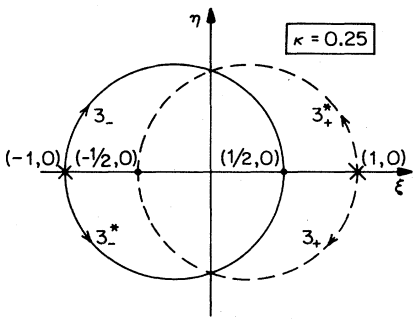

FIG. 6. Trajectories for the nontopological Rajaraman kink ($\kappa=0.25$).

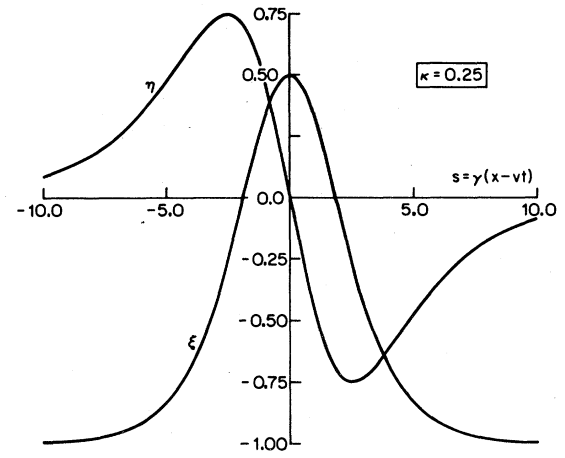

FIG. 7. Waveform of the 3_ (Rajaraman) kink in its rest frame.

Subbaswamy and Trullinger[43] (ST) have noted, however, that the Rajaraman kink ($\kappa=\frac{1}{4}$) energy instead satisfies the remarkable relation

$$E_3(0)=E_1(0)+E_2(0). \tag{5.5}$$

Moreover, ST have found numerical solutions for other κ values between 0 and 1 which are similar to the Rajaraman kink solution for $\kappa=\frac{1}{4}$; a few trajectories for 3_ numerical solutions are shown in Fig. 8 (taken from their paper[43]). From their numerical solutions ST found that the energy $E_3(0)$, of the class-three nontopological kink satisfies Eq. (5.5) for *all* κ values between 0 and 1.

This very interesting energy "sum rule" [Eq. (5.5)] has the immediate consequence that the energy of the class-three nontopological kink is greater than that of two topological class-two kinks, since

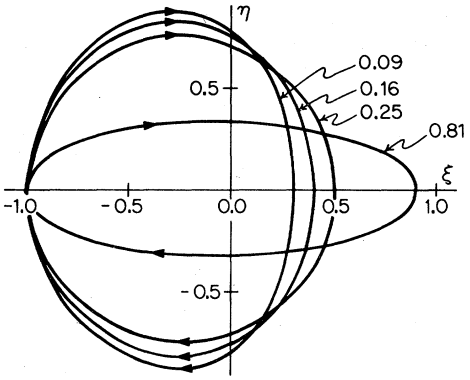

FIG. 8. Nontopological 3_ kink trajectories for various values of κ (taken from Ref. 43). Note that these trajectories intersect the ξ axis at $(\sqrt{\kappa},0)$.

$E_1(0) > E_2(0)$ for $\kappa < 1$. This strongly suggests that the nontopological kinks of the Rajaraman type are unstable to decay into two appropriate class-two topological kinks. ST have performed a numerical analysis[44] of the linear stability of these nontopological kinks and found that they are indeed *unstable*. A possible decay channel for a type 3_ kink, for example, would be

$$3_- \rightarrow 2_+ + 2_-^* + X \ , \tag{5.6}$$

since the energy remaining after the production of two class-two kinks is just

$$\Delta E = E_3(0) - 2E_2(0)$$
$$= E_1(0) - E_2(0) = E_X \quad (\kappa < 1) \ , \tag{5.7}$$

which is *precisely* the activation energy of the unknown excitation for $\kappa < 1$. This possibility suggests an indirect way of finding the X excitation numerically, namely, one could prepare a class-three kink, perturb it slightly and examine its decay products. This procedure is currently being carried out.[45]

Even if we suppose that such a numerical investigation will be successful in finding the X solution for $\kappa < 1$, it would remain to find the corresponding solution for $\kappa > 1$ where nontopological solutions of the Rajaraman type are not known. Moreover, it would be most beneficial to have *analytic* X solutions for a variety of purposes including the development of a kink-gas phenomenology analogous to the CKBT theory[4] and also for a closer examination of the statistical mechanics near the bifurcation point $\kappa = 1$ where E_X vanishes. The statistical mechanics results in Sec. IV have already suggested that the unknown excitation is nontopological. We now examine additional clues provided by these results which will hopefully aid in finding analytical solutions.

Information pertaining to the X kink trajectory in $\xi - \eta$ space can be obtained by noting that E_X arises in the calculation of the tunneling free energy via WKB tunneling integrals along specific paths in the elliptic coordinate system. When $\kappa < 1$, the path followed is a "radial" one ($u = u_\kappa \rightarrow u = 0 \rightarrow u = u_\kappa$) with $v = 0$ (or π). For $\kappa > 1$, the path is "angular" [e.g., $v = \cos^{-1}(\kappa^{-1/2}) \rightarrow v = 0 \rightarrow v = \cos^{-1}(\kappa^{-1/2})$] with $u = 0$. The corresponding paths in $\xi - \eta$ space are shown in Fig. 9, where they take the form of straight-line paths along the ξ axis. For example, if the starting minimum is $(\xi, \eta) = (1, 0)$, then the paths extends to $(\xi, \eta) = (\sqrt{\kappa}, 0)$ *and* back again. [It is interesting to note that the special point $(\sqrt{\kappa}, 0)$ is also the intersection point of the 3_ kink with the ξ axis for all $\kappa < 1$ (see Fig. 8).]

If we hypothesize that the paths depicted in Fig. 9 are indeed the trajectories followed by the possible X solutions, then it becomes immediately apparent that such solutions must be time dependent. To see this,[46] let us focus on the specific example of a possible nontopological kink solution for $\kappa < 1$ which follows the path $(1, 0) \rightarrow (\sqrt{\kappa}, 0) \rightarrow (1, 0)$. Setting $\eta = 0$ we have from Eq. (1.3a) that

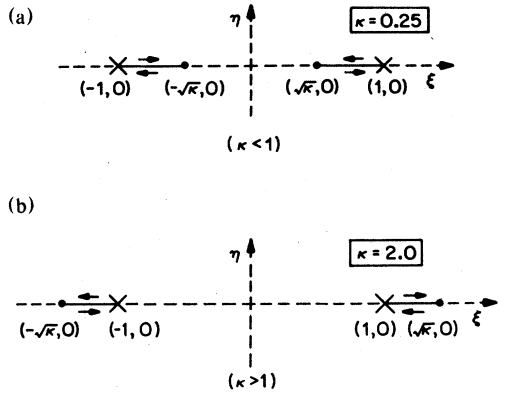

FIG. 9. Possible trajectories (solid lines) for the unknown excitation at the instant when all its energy (E_X) is potential. For both $\kappa < 1$ [part (a)] and $\kappa > 1$ [part (b)] the trajectories return to the originating potential minimum after reaching $|\xi| = \sqrt{\kappa}$.

$$\xi_{tt} = \xi_{xx} + \xi(1 - \xi^2) \ . \tag{5.8}$$

Without loss of generality we can place the origin ($x = 0$) at the center of the supposed kink. Obviously, ξ must have positive curvature at $x = 0$. In addition $\xi = \sqrt{\kappa}$ at $x = 0$ so that $\xi(1 - \xi^2) = \sqrt{\kappa}(1 - \kappa) > 0$. Thus at $x = 0$, Eq. (5.8) forces a positive value of ξ_{tt} and hence the solution must be time dependent if it follows the supposed trajectory. A similar argument applies for $\kappa > 1$.

An intrinsic time dependence of the unknown excitation implies that it has an additional degree of freedom over and above its translational degree of freedom. This additional degree of freedom is consistent with the extra power of $\beta^{-1/2} = (k_B T)^{1/2}$ in the prefactor of the tunneling free energy contribution of this excitation as compared to that for the relevant stable topological kink [see Eqs. (4.27) and (4.41)]. Also we note that a time variation of the excitation waveform suggests that the trajectories themselves may be time dependent, with those shown in Fig. 9 representing the trajectories at one instant of the motion when all of the energy is potential (recall that E_X arose in the calculation of the *configurational* free energy). Then $\xi_t = 0$ everywhere along the trajectories shown in Fig. 9.

VI. SUMMARY AND DISCUSSION

In this paper, we have described an analytic investigation of the low-temperature statistical mechanics of the two-component–kink-bearing MSTB Hamiltonian, using the transfer-operator method. The two-dimensional Schrödinger equation approximation to

the transfer-integral equation was found to separate into two one-dimensional eigenvalue equations by transforming to a "kink-path" coordinate system in which the paths followed by topological kinks in field $(\xi-\eta)$ space became constant-coordinate lines. The separated equations were solved analytically at low temperatures to obtain the lowest two eigenvalues of the transfer operator, which in turn yielded the configurational free energy and the correlation length for equal-time field fluctuations. In addition to the expected exponential tunnel-splitting contributions to these eigenvalues due to the known topological kinks, an unexpected exponential contribution was found which apparently is due to some sort of nontopological excitation. By relying on the correlation length for interpreting their numerical results, previous workers[31] overlooked this extra excitation (which does not influence the correlation length). The temperature dependence of the topological kink contribution to the configurational free energy is the same as that exhibited by familiar one-component kinks[4] and taking Eq. (4.45) as a hypothesis for the relation between kink density and correlation length led us to Eqs. (4.46) for the low-temperature densities of topological kinks. On the other hand, the additional factor of $(k_BT)^{1/2}$ appearing in the free energy contribution [Eq. (4.43)] of the unknown excitation suggests that this excitation has an additional degree of freedom which may be due to an intrinsic time dependence.

Besides the unexpected contribution of the unknown excitation to the free energy, one of the most fascinating features of our investigation involves what we have left undone, namely, the solution of the separated Schrödinger equations (3.13) for κ at and near the bifurcation point $(\kappa=1)$. As noted in the discussion following Eq. (4.44), the extreme flatness of the minima in the potentials, $U_1(u)$ and $V_1(v)$ [see Eqs. (3.15) and Fig. 4(b)] causes problems in developing a reliable tunneling formalism to obtain the lowest eigenvalues near $\kappa=1$. The solution of this problem should provide considerable insight into the nature of the kink bifurcation phenomena. In this context, we note the recent use[47–49] which has been made of this bifurcation effect in models of domain walls in uniaxial ferromagnets. We suspect an intimate connection between the unknown nontopological excitation and the bifurcation process in view of the fact that its energy vanishes at $\kappa=1$; perhaps it can be viewed as a *nonlinear* "soft mode" which plays a role in the phase-transition-like bifurcation.

We now turn to a discussion of the development of an ideal-gas phenomenology along the lines of Ref. 4. While the precise nature of the nontopological excitation remains unknown, a complete low-temperature phenomenology involving all of the nonlinear "modes" cannot be developed. However, if κ values near unity are avoided, so that the density of these unknown excitations can be assumed small enough to ignore their competition with the topological kinks for degrees of freedom, then a CKBT-type phenomenology[4] for the topological kinks should be possible. For $\kappa>1$, all the needed information concerning the small oscillations in the presence of a class-one kink is already known,[33] but unfortunately, the spectrum of small oscillations about a class-two kink is not yet known exactly and this prohibits a direct calculation of the class-two kink self-energy for $\kappa<1$ in the manner of CKBT. Nevertheless, it may be possible to extend the recent work by DeLeonardis and Trullinger[14,41] (for one-component systems) which does not require an explicit knowledge of these small oscillations. This more general approach is currently being investigated.[50]

Finally, we comment on the usefulness of kink-path coordinates for models other than the one (MSTB) considered above. To our knowledge, the only other model for which a transformation to kink-path coordinates has been successful in separating the 2D Schrödinger equation is the fourfold anisotropic model described by Subbaswamy and Trullinger[36] (ST). For a special value of their anisotropy parameter $(\lambda=3)$, the kink trajectories are known analytically (straight lines) and a transformation[51] to kink-path coordinates leads to two identical 1D Schrödinger problems involving the familiar ϕ-four potential whose lowest eigenvalues are known analytically.[8,41] However, for $\lambda\neq 3$, the kink trajectories are not known analytically.[36] ST have shown that they are *not* conic sections and as a consequence we consider it unlikely that the 2D Schrödinger equation is separable for $\lambda\neq 3$ even if analytic kink paths are eventually found.

Even though the use of kink-path coordinates may not lead to separation of the 2D Schrödinger equation for general two-component models, we nevertheless note that the kink trajectories must play a fundamental role in the interpretation of the low-temperature free energy and correlation length, and statistical mechanical investigations which utilize these trajectories are likely to provide much more insight than brute-force numerical methods.

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