Dirac chains in the presence of hairpins

Arkady L. Kholodenko[1,2] and Thomas A. Vilgis[1]
[1]*Max-Planck-Institut für Polymerforschung, P.O. Box 3148, D-55021 Mainz, Germany*
[2]*375 H.L. Hunter Laboratories, Clemson University, Clemson, South Carolina 29634-1905**
(Received 5 December 1994; revised manuscript received 25 May 1995)

We study semiflexible polymers of arbitrary stiffness subject to nematic and non-nematic elongation forces. The presence of nematic forces is found to cause the formation of hairpins. [A hairpin is an immediate return (or a sharp bend) of a chain in the nematic ordering field.] An analysis of the path integrals for semiflexible (Dirac) chains with these elongational forces indicates that the distribution functions describing these induced hairpins satisfy the Whittaker-Hill (WH) equation in two dimensions. The same equation describes hairpins in three dimensions if (and only if) the Dirac monopole term is included in the corresponding path integral. The solutions of the WH equation indicate that the non-nematic stretching force can only have discrete values corresponding to the sequential destruction of hairpins. This discreteness disappears when the nematic force is absent, as demonstrated in previous work [A. Kholodenko and T. Vilgis, Phys. Rev. E **50**, 1257 (1994)]. We also indicate how the hairpin problem is related to other statistical mechanical problems of interest: commensurate-incommensurate transitions, quantum spin chains, Landau-Lifshitz equation, rotational Brownian motion, strings with rigidity, etc.

PACS number(s): 61.41.+e, 11.10.−z, 75.10.Jm

I. INTRODUCTION AND SUMMARY

The elastic response of polymeric materials has been considered in great detail during the last few decades. The basic idea was to study a weakly interacting ensemble of (crosslinked) polymers where the elastic response of the entire ensemble can be mapped onto the behavior of a single chain. In most studies the single chain has been modeled by a Gaussian random walk with *no* intrinsic flexibility. Real chains are non-Gaussian and local stiffness is important. Especially in liquid crystalline polymers the stiffness is so large (at certain temperatures) that the persistence length could be of the order of the chain size. In this limit the Dirac propagator can be used for such a chain [1].

Recently, we have studied the elastic response of the Dirac chain to elongation forces of non-nematic origin [1], i.e., for the ordering field-free case. Dirac chains are believed to reproduce correctly conformational properties of semiflexible polymers of arbitrary stiffness: from random coils to rigid rods (e.g., see [2], and references therein). Use of the Dirac chains complements the results of classical elasticity theory of simple ideal Gaussian chains and networks [3] which are valid in the limit of small bending energies. In [1] we found that the elongation as a function of non-nematic force for the Dirac chain is described in terms of the same type of Langevin function which was derived earlier for the random flight models [3]. Stretching of polymer chains subject to hydrodynamic elongational flow or magnetic-type forces has been studied experimentally in [4], while stretching due to both nematic and non-nematic forces simultaneously does not seem to have been experimentally investigated before. This type of stretching was recently discussed theoretically in [5] in connection with de Gennes's hairpin problem [6] and earlier by Jähnig [7]. A hairpin is the immediate return (or a sharp bend) of the chain in the nematic ordering field. Hairpins were observed experimentally quite recently in the absence of non-nematic forces [8]. Theoretically, the combination of nematic and non-nematic stretching superimposed with confinement of the polymer solution between the parallel plates was also recently considered in [9] without use of path integrals, while in [10] the conformational statistics properties of single chains of arbitrary flexibility were studied in confined geometries by using the Dirac propagator. In this paper we study the Dirac chain subject to nematic and non-nematic force perturbations. As a result, the problem of hairpins is being reexamined and many new and unexpected aspects of the hairpin problem are discovered and discussed in some detail. These single chain results are required for development of a theory of elasticity of networks of semiflexible chains which is left for future investigation.

This paper is organized as follows. In Sec. II we provide general background and a statement of the problem. Here we demonstrate that the existing hairpin model of Gunn and Warner [5] can be rigorously obtained from the one-dimensional (1D) Ising model in an external "magnetic" field which, in turn, is also a discrete model analog for the $(1+1)$-dimensional Dirac propagator independently obtained in [11]. Because the 1D Ising model is isomorphic to the quantum mechanical double well problem [12], the problem of hairpins is analogous to the problem of domain wall formation along the one-dimensional Ising chain [13,14]. With respect to the

*Permanent address.

Dirac chain, the problem arises: How is the elasticity parameter (i.e., the inverse of the mass of the Dirac "particle" [11]) renormalized in the presence of the nematic environment? With respect to the existing continuum path integral treatments [13,15,16] of semiflexible chains the further problem arises: Under what conditions are these integrals reducible to that for the 1D Ising model? Finally, we investigate what (if any) is the relationship between these path integrals and those for the Dirac propagator. In Sec. III we discuss an analogy between the existing path integrals for hairpins and that for the quantum and classical *XXZ* chains. Because the quantum *XXZ* chain is isomorphic to the massive. Thirring model [17,18], which is the $(1+1)$-dimensional massive Dirac field with quartic self-interaction, we conclude that the de Gennes hairpin problem can be, in principle, solved exactly, because the massive Thirring model admits an exact solution [17]. The exact solution for the Thirring model is, however, not too physically illuminating. Therefore in Sec. IV we consider a simplified version of an *XXZ* chain based on the existing treatments of quantum chains in terms of two-dimensional nonlinear σ models [19] with the Chern-Simons (CS) term. The high temperature semiclassical limit of these models corresponds (without the CS term) to the existing path integrals for the semiflexible chains (in the absence of nematic coupling). The addition of the CS term converts these integrals to those which are related to the Dirac propagator [20]. To explain the physics associated with addition to the CS term, we consider in some detail a planar version of such path integrals for which the calculations could be made especially transparent. At the classical level the CS term is a total "time" derivative and reduces in two dimensions to a winding number (which we discussed earlier in [21]) while at the quantum path integral level it leads to a rigidification of the polymer chain. Although the rigidity of the chain can be controlled, without the CS term, with help of the existing Kratky-Porod-type path integrals for the semiflexible chains [22], its role becomes indispensable for the hairpin problem. In Sec. V we treat the planar problem with the CS term to illustrate this point but this time we include terms responsible for the nematic and non-nematic stretching. We show that the inclusion of the nematic term leads in the planar case to a classical action which is *identical* to a standard model of commensurate-incommensurate (*C-I*) transitions [23,24]. This connection is only possible if the CS term is present, which explains why the fermionic analogy in the theory of *C-I* transitions is used. Additional inclusion of the non-nematic stretching factor leads to physically unexpected effects. The Schrödinger-like equation corresponding to this two-dimensional path integral is known in the mathematical literature as the Whittaker-Hill equation [25], while without non-nematic stretching the equation is of Mathieu type [26]. Both equations are also of the Hill type [27] and therefore the Floquet theory can be used to solve them [28]. At the very elementary level (without non-nematic stretching) the Taylor series expansion of the nematic term produces a double well Schrödinger-type one-dimensional equation which, as indicated above, is isomorphic to the 1D Ising model, and therefore, to hairpins. If, however, we do *not* use the Taylor series expansions, then *even if initially the CS term in the action was absent, it reappears in calculations in the form of the Floquet exponent.* Moreover, an addition of the non-nematic stretching term causes nontrivial effects such as *quantization of the non-nematic stretching force.* This quantization physically is associated with the fact that hairpins have a well defined energy so that their destruction is possible only discontinuously. Indeed, it is intuitively clear that stretching of a chain with hairpins in a nematic environment does not change its nematic energy as long as no hairpin is dissolved. Moreover, because the Mathieu-type equations exhibit chaotic behavior [29], the values of Floquet exponents can also have discontinuous jumps depending upon the strength of the nematic coupling [30]. We interpret these jumps in terms of the nematic-isotropic transition. The extent to which this two-dimensional picture survives in three dimensions is discussed in Sec. VI. We demonstrate that all two-dimensional results remain unchanged *if and only if* the CS term is present in the action. Such path integrals with the CS term and in the absence of stretching couplings correspond to the Schrödinger-like equation for the Dirac monopole [31].

In Sec. VII we include the Dirac monopole problem in a more general type of theories. This is motivated by our interest in nonperturbative (i.e., different from that presented in [30]) methods of treatment of the hairpin problem. We demonstrate at the classical level that the mathematical equivalent of the hairpin problem without the monopole term was solved *exactly* in 1859 [32] and with the monopole term as early as 1892 [33]. These mathematical problems were rediscovered late in the 20th century in connection with the exactly integrable systems. The quantum versions of these results are briefly discussed as well in this section. Finally, in Sec. VIII we briefly show how the hairpin problem occurs in other areas of physics, thus demonstrating its central role in recent developments ranging from quantum groups to hydrodynamics of suspensions of aspherical particles.

II. BACKGROUND AND STATEMENT OF THE PROBLEM

Let $G(\mathbf{R},N)$ be the end-to-end distribution function. Following de Gennes [34], the generating function $Z(f)$ for the polymer chain of length N in the field of force F is given by

$$Z(\mathbf{f})=\int d\mathbf{R}\, G(\mathbf{R},N)e^{\mathbf{f}\cdot\mathbf{R}}\ , \tag{2.1}$$

where $\mathbf{f}=\mathbf{F}/k_BT$ ($k_BT=\beta^{-1}$ is the thermal energy). According to Eq. (2.1), if $G(\mathbf{k},N)$ is the Fourier transform of $G(\mathbf{R},N)$, then $Z(f)$ is obviously related to $G(\mathbf{k},N)$ via replacement $\mathbf{f}\Longrightarrow i\mathbf{k}$. The function $G(\mathbf{k},N)$ can be calculated for chains of arbitrary stiffness using the analogy with the directed random walk problem in $1+1$ dimensions. This problem happens to be related to the propagation of a Dirac particle in $(1+1)$ dimensions, as indicated before by Feynman. (The details of the derivation can be found in [11].) The propagator equals

$$\mathbf{G}(k,N)=2\cosh(mEN)+\frac{2}{E}\sinh(mEN) , \tag{2.2a}$$

where m is related to the stiffness parameter as explained after Eq. (2.9), N is the chain length, and $E^2=1+k^2/2m^2$.

In [5] the dielectric response of a semiflexible polymer chain was considered within the framework of the hairpin model suggested by de Gennes [6]. The authors had obtained for $Z(\mathbf{f})$ the following result:

$$Z(\mathbf{f})=2\left[\cosh(AN)+\frac{\varphi}{A}\sinh(AN)\right] , \tag{2.2b}$$

where $A^2=\nu^2+\varphi^2$, $\nu=\mathbf{f}\cdot\boldsymbol{\ell}$, $\varphi=\exp(-h/k_BT)$, with h being the hairpin energy. The parameter ℓ is indirectly related to the mean hairpin density $\bar{n}$ defined by

$$\bar{n}=-k_BT\frac{\partial}{\partial h}\ln Z \tag{2.3}$$

so that $N/\bar{n}=1/\varphi$ [e.g., see Eq. (16) of [6]]. The bending energy ε of the continuous semiflexible chain is required to be related to ℓ via

$$\ell=\frac{1}{2}\frac{\varepsilon}{h}\left[\frac{k_BT}{h}\right] . \tag{2.4}$$

To analyze these results, the following observations are helpful. By taking the Laplace transform of Eq. (2.2) its physical meaning becomes more transparent. To do so, we rewrite $AN=\ell N\sqrt{\mathbf{f}^2+(\bar{n}/N)^2}$ taking into account that, according to [5], $(\mathbf{f}\cdot\boldsymbol{\ell}=f\ell)$. Now let $L\equiv\ell N$ and $m=\bar{n}/N$ be the mean number of hairpins per unit length, then the Laplace transformed version of Eq. (2.2b) can be written as

$$\frac{1}{2}L(Z(\mathbf{f}=i\mathbf{k}))=\frac{s+m}{\mathbf{k}^2+s^2-m^2} , \tag{2.5}$$

where s is the Laplace variable conjugate to L and Eq. (2.5) is written in $(d+1)$-dimensional form. In the papers [2,10,11] we have demonstrated that the right-hand side of Eq. (2.5) can be obtained from the Euclidean version of the Dirac propagator $D_E(\mathbf{k},s)$ given by

$$D_E(\mathbf{k},s)=\frac{-i}{\not{k}+\mu}=i\frac{\not{k}-\mu}{k^2+\mu^2} , \tag{2.6}$$

were $\not{k}=\sum_\alpha\gamma^\alpha k_\alpha$, $k^2=\mathbf{k}^2+s^2,\gamma^\alpha$ are Euclidean-type Dirac matrices [35] so that $\{\gamma^\mu,\gamma^\nu\}=2\delta^{\mu\nu}$ and $\mathrm{Tr}\gamma^\mu=0$ but $\mathrm{Tr}(\gamma^\mu)^2=-1$. To obtain the right-hand side of Eq. (2.5) from Eq. (2.6) the connection between the continuous and the discrete versions of the Dirac propagators is the most helpful. As discussed in [11], and summarized in Eq. (2.2a), the lattice version of the Dirac propagator is obtained only if the proper averaging over the initial directions and summation over the final directions of the walk is made (as it is done in the continuous limit for the Dirac particle [36]). In the continuous limit the polarization density matrix $\rho=\frac{1}{4}(\mathbf{I}+a_\mu\gamma^\mu)$ is used with the property $\mathrm{Tr}\rho=1$ and a_μ could be assigned to properly account for the initial and the final states. By choosing $\rho=\frac{1}{4}(\mathbf{I}+i\gamma^4)$, multiplying both sides of Eq. (2.6) by ρ, taking the trace, and writing $\mu\Longrightarrow im$ we obtain Eq. (2.5). We would like to note that to obtain Eq. (2.5) it is actually sufficient to consider only the $1+1$ version of the Dirac propagator because in [5] the hairpin problem was treated only in one spatial (along the electric field) and one "time" (contour position along the chain) dimensions. Because of this, further simplifications are possible. For instance, Eq. (2.2b) is directly related to the partition function of the 1D Ising model in the presence of constant "magnetic" field. This can be seen by comparison between Eqs. (2.2a) and (2.2b). They coincide exactly if the following identification is made:

$$A^2\Longleftrightarrow m^2E^2 , \tag{2.7}$$

$$\nu^2\Longleftrightarrow\frac{k^2}{2} , \tag{2.8}$$

$$\varphi^2\Longleftrightarrow m^2 . \tag{2.9}$$

Equation (2.2a), obtained in [11], using the discrete analog of the Dirac propagator; moreover, it is the partition function for the 1D Ising model in a magnetic field. According to [11], the mass parameter m is related to the trans-gauche bending energy j as $i\hat{\varepsilon}m=\exp(-2j)$ where $\hat{\varepsilon}$ is of the order of the effective monomer length. The presence of a complex number i causes no problem because only m^2 enters into E^2 defined by Eq. (2.2a). Alternatively, we may use m instead of im but change k into ik as discussed after Eq. (2.1). In any case we obtain the simple relation

$$m=\frac{1}{\hat{\varepsilon}}\exp(-2j) . \tag{2.10}$$

This result formally coincides with de Gennes, Eq. (12) of [6], if we identify our $\hat{\varepsilon}$ with ℓ, which is indeed useful since "Quantitatively the chain is expected to behave as a succession of rigid pieces, each of length ℓ" [6]. Thus the variable m acquires the meaning of the inverse of the average distance between the hairpins. This distance can also be obtained using Eq. (2.3) so that the parameter ℓ introduced earlier coincides with that proposed by de Gennes.

By reformulating de Gennes's hairpin problem in terms of the Dirac propagator several questions remain open. First, as was already suggested by de Gennes, the correlation length ℓ, which is an effective persistence length, is related to the chain bending energy, on one hand, and to the coupling energy between the chain alignment and the nematic matrix alignment, on the other hand. Obviously, the conformation of a given chain can be anywhere between the rigid rod and the random coil limit depending upon its local bending energy as compared to the thermal energy k_BT and on the bending energy renormalization due to the presence of other polymers (or nematic matrix). The use of a single chain Dirac propagator does not allow us to address the above issue of renormalizability. Therefore we arrive at the second question: how can a theory of conformational properties of a single semiflexible chain be developed so that it can account for the effects of the presence of other chains? Although we have provided the general answer to this question already in [37], here we would like to specialize on a particular case of a semiflexible polymer embedded in an already existing nematic environment. Such a problem was considered by several authors [5,9,13,14] in the past but no attempt has been made to obtain the hairpin results from more sophisticated path integral treatments. Here we would like to provide such connections in order to address the problems posed above.

To do so, several remarks have to be made. Because the $(1+1)$-dimensional Dirac propagator can be obtained from the one-dimensional Ising model [11], the same is true for Eqs. (2.2a) and (2.2b). At the same time, it is known that the 1D Ising model is isomorphic to a two-level quantum mechanical system [12], e.g., to a double well problem. Thus more sophisticated path integrals [13,15,16] should be reducible to Ising-like ones that reproduce the double well behavior. This was noticed in [13]. The result, Eq. (2.2b), also differs in one important aspect from the existing path integral treatments. This is so because Eq. (2.2) describes the conformations of semiflexible polymers in the nematic matrix in the presence of hairpins, caused by polymer-nematic interactions *and, in addition,* in the presence of the external electric field, which plays the same role as the magnetic field in the Ising model or the nonzero momentum in the case of the Dirac propagator problem, e.g., see Eq. (2.8).

In our previous work [1], we had considered the elastic response of the Dirac chain to the external elongating fields in the absence of other chains, e.g., nematic matrix. We had obtained a closed form analytic result for this case. At the same time, the existing path integral treatments of hairpins *do not* include the external elongating fields, except Ref. [7]. References [5,14] include the elongating fields but without use of path integrals. In the language of the Ising model the presence of the elongating field is attributed to the magnetic field which may, in principle, be different at each lattice site. The presence of the field removes the characteristic degeneracy intrinsic for the double well and the difference in treatments for nonzero fields versus that of zero fields is of the same nature as the difference in treatments of the first and the second order phase transitions in statistical mechanics. In the remainder of this paper we shall study different path integral models of semiflexible chains that account for both the nematic interactions and for the elongation forces.

III. THE ANALOGY WITH *XXZ* QUANTUM SPIN CHAINS

Traditionally, semiflexible polymers are being described by the Kratky-Porod-type propagator given by

$$G(\mathbf{u}_f,\mathbf{u}_i;N)=\int_{\mathbf{u}(0)=\mathbf{u}_i}^{\mathbf{u}(N)=\mathbf{u}_f}[\mathbf{u}(\tau)]\delta(\mathbf{u}^2-1)\times\exp\left\{-\frac{\kappa}{2}\int_0^N d\tau\left[\frac{d\mathbf{u}}{d\tau}\right]^2\right\}. \tag{3.1}$$

In [38] it was shown that Eq. (3.1) can also be interpreted as the partition function for the classical one-dimensional Heisenberg model. Following Refs. [39,40], the partition function for this model can be written as

$$Z_N=\int\prod_{i=0}^{N}\frac{d\Omega_i}{4\pi}\exp\left[K\sum_{i=1}^{N}\mathbf{s}_i\cdot\mathbf{s}_{i-1}\right]. \tag{3.2}$$

Here $d\Omega_i$ is an element of solid angle for the unit vector s_i. Equation (3.1) is reduced to (3.2) if instead of the continuum version the discrete version of Eq. (3.1) is considered taking into account the unit sphere constraint $\mathbf{u}^2=\mathbf{u}\cdot\mathbf{u}=1$, as explained in [37]. The partition function, Eq. (3.2) can be easily calculated so that the correlation function [37–40] is given by

$$\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle=\frac{1}{n}\left[\frac{I_{n/2}(K)}{I_{n/2-1}(K)}\right]^{|i-j|}, \tag{3.3}$$

where n is the number of components of the vector $\mathbf{s}_i$ (usually in 3D physics $n=3$ is being used, not to be confused with the self-avoiding walk model, i.e., $n=0$), and $I_n(x)$ is the modified Bessel function. As it was shown in [37,40], for the physically relevant range of values of K, we can use the asymptotic limit of Eq. (3.3),

$$\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle\approx\exp\left[-\frac{n-1}{2K}|i-j|\right]. \tag{3.4}$$

The situation changes dramatically in the presence of a constant field $\mathbf{f}$, i.e., if we replace the exponent in Eq. (3.2) by the following expression:

$$H=K\sum_{i=1}^{N}\mathbf{s}_i\cdot\mathbf{s}_{i-1}+\sum_{i=1}^{N}\mathbf{f}\cdot\mathbf{s}_i. \tag{3.5}$$

In this case Z_N and the correlation functions cannot be calculated exactly [40]. At the same time, in previous work [37] such exact calculation was performed for polymer chains of arbitrary stiffness using the Dirac propagator. In view of this, let us consider once again the modified partition function Z_N, upon rewriting the action in the exponent in the form given by

$$\hat{H}=K\sum_{i=1}^{N}\mathbf{s}_i\cdot\mathbf{s}_{i-1}-g\sum_{i=1}^{N}s_i^zs_{i-1}^z\equiv\sum_{i=1}^{N}(J_xs_i^xs_{i-1}^x+J_ys_i^ys_{i-1}^y+J_zs_i^zs_{i-1}^z), \tag{3.6}$$

where $J_x=J_y=K$ and $J_z=K-g$. The model described by such action is known in the literature as the *XXZ* model [18,23,24]. Let us study the continuum limit of this model. To this purpose it is sufficient to write the expansion for $\mathbf{s}_i$ [41],

$$\mathbf{s}_{i+1}=\mathbf{s}_i+a\frac{d\mathbf{s}_i}{dx}+\frac{a^2}{2}\frac{d^2\mathbf{s}_i}{dx^2}+\cdots, \tag{3.7}$$

where a is the lattice spacing. Use of Eq. (3.7) in Eq. (3.6) and replacement of sums by integrals produces in the continuum limit

$$S=\frac{1}{2}\int_0^N d\tau\left[\kappa\left[\frac{d\mathbf{s}}{d\tau}\right]^2+\tilde{g}(s^z)^2\right], \tag{3.8}$$

where the constants κ and $\tilde{g}$ are related to the coupling parameters K and K-g. The model based on the action S given by Eq. (3.8) was studied recently in connection with the hairpin problem [13]. It was argued (without detailed proof), that it exhibits 1D Ising-like behavior and thus it provides an adequate description of hairpins. In connection with Eq. (3.8), it is useful to provide the alternative versions of the hairpin actions for the latter purpose. For example, in [15,16] instead of Eq. (3.8), an equivalent expression proposed by Warner, Gunn, and Baumgärtner (WBG) was used,

$$S_{\rm WGB}=\frac{1}{2}\int_0^N d\tau\left[\kappa\left[\frac{d\mathbf{s}}{d\tau}\right]^2+\tilde{g}[3(s^z)^2-1]\right] . \quad (3.9)$$

This result was earlier discussed in [7], where an even more general action was considered:

$$S_J=S_{\rm WGB}+f_z\int_0^N d\tau\, s^z , \quad (3.10)$$

where f_z is the z component of the field $\mathbf{f}=(0,0,f_z)$.

The action, Eq. (3.10), describes the elongation due to the external forces as well as to the presence of the nematic environment as discussed in Sec. II. Because Eqs. (3.8)–(3.10) come from their discrete counterparts, given by Eqs. (3.5) and (3.6), we return to these equations once again. The quantum spin version of the model given by Eq. (3.6) is known as the XYZ model [18], while for $J_x=J_y\neq J_z$ the model is known as XXZ [18,23,24]. For completeness, we would like to provide a few details which connect these kinds of models with Dirac fermions. Given that for the quantum spin operators s_i.

$$(s_i^x)^2+(s_i^y)^2=s_i^+s_i^-+s_i^-s_i^+ ,$$

it can be shown [18] that the Hamiltonian for the XYZ model can be written as

$$\hat{H}=\sum_{i=1}^N[(s_{i-1}^+s_i^++s_{i-1}^-s_i^+)+\Gamma(s_{i-1}^+s_i^++s_{i-1}^-s_i^+) +2\Delta(s_{i-1}^zs_i^z-\tfrac{1}{4})] , \quad (3.11)$$

where the coupling constants Γ and Δ are related to J_i in a known way.

We next introduce the spin Fourier transforms

$$s_k^+=\sum_{n=1}^N e^{ikn}s_n^+,\quad s_k^z=\sum_{n=1}^N e^{ikn}s_n^z ,$$

such that $s_k^-=(s_k^+)^*$, where $*$ denotes complex conjugation. Finally, the creation-annihilation operators are introduced via

$$s_k^-s_k^+\to Na_k^\dagger a_k-\sum_{p,p'}a_k^\dagger a_{p+p'-k}^\dagger a_p a_{p'} ,$$

$$s_k^zs_k^z\to\sum_k a_k^\dagger a_k+\sum_{p,p'}a_{p-k}^\dagger a_{p'+k}^\dagger a_p a_{p'} ,$$

which in continuum limit go into the operatorlike wave functions ψ, $\psi^\dagger$, etc. as it is explained in [18]. After all this algebra is done, we finally obtain for the XXZ case the self-interacting Dirac Hamiltonian known as the massive Thirring model [18]. It is given by the Hamiltonian of the following type:

$$\hat{H}_T=\int_0^L dx\,\psi^\dagger(x)\left[-i\alpha\frac{\partial}{\partial x}+\beta m\right]\psi(x) +4\Delta\int_0^L dx\,\psi_1^\dagger(x)\psi_1(x)\psi_2^\dagger(x)\psi_2(x) , \quad (3.12)$$

where 2×2 Dirac matrices are given by

$$\alpha=\begin{bmatrix}1&0\\0&-1\end{bmatrix}=\sigma_z,\quad \beta=\begin{bmatrix}0&-i\\i&0\end{bmatrix}=\sigma_x$$

and σ_z and σ_x are the usual Pauli matrices. The parameters m and Δ are related to K and g in a known way [18] and L is the size of the system (in x direction). Statistical mechanics can now be developed in $1+1$ dimensions and the semiclassical (high temperature) limit of the massive Thirring model can be obtained exactly since the massive Thirring model is exactly integrable in $1+1$ dimensions [17], so that the classical model based on Eq. (3.8) is also exactly solvable. We shall discuss what all this actually means below in Secs. V–VII, while in the meantime we only would like to note the following. First, $1+1$ free (i.e., $\Delta=0$) Dirac fermions coming from Eq. (3.12) are in one to one correspondence with Dirac fermions of Sec. II. The presence of interactions yields a mass renormalization, whence it is possible to account for the effects of nematic environment by studying the mass renormalization effects. This will provide us with answers to the questions posed in Sec. II. Second, as in Sec. II, the $1+1$ version of the Dirac propagator can be replaced by the $3+1$ version (this simply will account for the transversal degrees of freedom of the polymer chain as discussed, for example, in [11,13,37]). The field-theoretic methods leading to renormalization and critical exponents for a self-interacting Dirac field in dimensions $2<d\leq4$ were recently discussed in [42–44]. The complete development of the theory of nematic order using field-theoretic methods is rather cumbersome and therefore we plan to investigate its physical implications in a separate publication. For the moment, we shall concentrate on the alternative methods of studying this problem.

IV. THE ANALOGY WITH THE TWO-DIMENSIONAL NONLINEAR σ MODEL

It has been known for some time that the statistical mechanics of quantum spin chains can be successfully described in terms of the classical path integrals known as a nonlinear σ models [19]. In fact, Eq. (3.1) is already a special type of σ model. More generally, the functional integral for the nonlinear σ model can be written as [12]

$$I=\int D(\mathbf{u}(\mathbf{x}))\prod_x\delta(\mathbf{u}^2(\mathbf{x})-1)\exp\{-S[\mathbf{u}]\} , \quad (4.1)$$

where

$$S[\mathbf{u}]=\frac{1}{2}\kappa\int d^2r\,\partial_\mu\mathbf{u}\partial^\mu\mathbf{u}+\frac{i\Theta}{8\pi}\int d^2x\,\varepsilon^{\mu\nu}\mathbf{u}\cdot\partial_\mu\mathbf{u}\partial_\nu\mathbf{u} . \quad (4.2)$$

The Θ term is formally the total derivative [19] and plays no role at the classical level while at the quantum level this is no longer the case. We demonstrated in an earlier work [21] that inclusion of the winding number (also the total "time" derivative) in the corresponding Gaussian path integrals leads to nontrivial effects at the quantum level and we find this is also true here. It was also shown in previous work [1] that the one-dimensional version of the nonlinear σ model including the Θ term changes the propagator, Eq. (3.1), from bosonic to fermionic (Dirac-like) so that the propagator for the Dirac chain can be effectively written as [45]

$$G^D(\mathbf{r},\mathbf{r}';\mathbf{u}_f,\mathbf{u}_i;N)=\int_{\mathbf{u}(0)=\mathbf{u}_i}^{\mathbf{u}(N)=\mathbf{u}_f} D(\mathbf{u}(\tau))\delta(\mathbf{u}^2-1)\delta\left[\mathbf{r}-\mathbf{r}'-\int_0^N d\tau\,\mathbf{u}\right] \times\exp\left\{-\frac{1}{2}\kappa\int_0^N d\tau\left[\frac{d\mathbf{u}}{d\tau}\right]^2+i\int_0^N d\tau\,\mathbf{A}(\mathbf{u}(\tau))\cdot\frac{d\mathbf{u}}{d\tau}\right\}, \tag{4.3}$$

where $A(\mathbf{u}(\tau))$ is defined [19,20] as

$$\int_0^N d\tau\,\mathbf{A}(\mathbf{u}(\tau))\frac{d\mathbf{u}}{d\tau}=\Theta\int_0^N d\tau\int_0^N d\tau'\mathbf{u}\cdot\left[\frac{\partial\mathbf{u}}{d\tau}\wedge\frac{\partial\mathbf{u}}{d\tau'}\right]. \tag{4.4}$$

The above Θ term is written in a form given by Eq. (4.4) for a special case of closed paths. If the paths are open, some insignificant changes in the Θ term should be made [45]. We ignore these changes, however, because they are not going to affect our results for long chains. Following Polyakov [20] and others [37,46], we shall call the term

$$C(\mathbf{u}(\tau))=\int_0^N d\tau'\mathbf{u}\cdot\left[\frac{d\mathbf{u}}{d\tau}\wedge\frac{d\mathbf{u}}{d\tau'}\right] \tag{4.5}$$

the torsion of the curve. In our previous work [37] we have emphasized that the torsion term is always nonzero for *nonplanar* curves and is zero for planar. Hence this term should always be present in the path integral action. The reason it is usually ignored lies in the fact that it is a total "time" derivative and at the classical level it can be discarded. Recently, however, this term was considered at the classical level in connection with problems related to the elasticity of cholesterics in [47], while in [31] and later in [48] it was shown that the path integral, Eq. (4.3), corresponds to the propagator for the nonrelativistic charged particle in the presence of the magnetic Dirac monopole. We shall provide more details to these statements below in Sec. VI. In the meantime, it is useful to consider a slightly simpler problem in order to understand the underlying physics better.

Let us first consider the planar rotator whose Hamiltonian $\hat{H}_\phi$ is given by

$$\hat{H}_\phi=-\frac{1}{2}\kappa\frac{d^2}{d\phi^2}. \tag{4.6}$$

The dimensionless eigenvalues E_l of the corresponding Schrödinger equation are given by $E_l=\frac{1}{2}l^2$, $l=0,\pm1,\pm2,\ldots$, while the eigenfunctions are $\Psi_l=\sqrt{1/2\pi}\exp(il\phi)$. Following Ref. [49], let us further generalize the problem. First notice that the eigenfunctions ψ_l usually obey the standard periodic boundary condition, i.e., $\Psi_l(\phi+2\pi)=\Psi_l(\phi)$. More generally we would require

$$\Psi_l(\phi+2\pi)=\exp(-i\theta)\Psi_l(\phi), \tag{4.7}$$

where $0\le\theta<2\pi$, and this leads to the wave function

$$\Psi_l(\phi)=\left[\frac{1}{2\pi}\right]^{1/2}\exp\left[i\left[l-\frac{\theta}{2\pi}\right]\phi\right], \tag{4.8}$$

while the energy eigenvalues are changed into

$$E_l=\frac{1}{2}\left[l-\frac{\theta}{2\pi}\right]^2. \tag{4.9}$$

As we discussed in our previous work, Ref. [21], it is more advantageous sometimes to replace the boundary conditions, Eq. (4.7), by the standard periodic ones at the expense of replacing the simple Hamiltonian, Eq. (4.6), by

$$\hat{H}^\theta_\phi=\kappa\frac{1}{2}\left[i\frac{d}{d\phi}+\frac{\theta}{2\pi}\right]^2. \tag{4.10}$$

At the classical level this yields the Lagrangian

$$L_\theta=\kappa\frac{1}{2}\left[\left[\frac{d\phi}{dt}\right]^2+\frac{\theta}{2\pi}\frac{d\phi}{dt}\right]. \tag{4.11}$$

Evidently, the last term is a total time derivative and thus can be discarded. This is not exactly the case at the quantum level in view of Eq. (4.9).

The corresponding Euclidean path integral corresponds to the problem of diffusion on a unit sphere (circle in two dimensions). It can be written as [37,38]

$$G(\mathbf{u}_f,\mathbf{u}_i;N)=\int_{\mathbf{u}(0)=\mathbf{u}_0}^{\mathbf{u}(N)=\mathbf{u}_f}(\mathbf{u}(\tau))\delta(\mathbf{u}^2-1)\exp\left\{-\frac{1}{2}\kappa\int_0^N d\tau\left[\frac{d\mathbf{u}}{d\tau}\right]^2+i\frac{\theta}{2\pi}\int_0^N d\tau\frac{d}{d\tau}\tan^{-1}\left[\frac{u_y}{u_x}\right]\right\} \tag{4.12a}$$

and it differs from that discussed in our earlier work [21] only by an additional δ constraint. Without this constraint, the path integral, Eq. (4.12a), describes the Brownian motion on the plane in the presence of a hole while the presence of this constraint constrains the random walk to the circle. In the planar case, the θ term reflects the strengths of interactions between the Brownian particle and the hole while in the case of a circle this term represents the degree of mapping of a circle into itself and is responsible for the change in statistics as we are about to demonstrate (we have also briefly discussed this fact earlier in [10,21]). In two dimensions we use θ instead of Θ.

To this purpose, let us introduce the generating function

$$\left\langle \exp\left[i\mathbf{p}\cdot\int_0^N \mathbf{u}(\tau)d\tau\right]\right\rangle = \mathfrak{J}\int_{\mathbf{u}_i=\mathbf{u}_f} D(\mathbf{u}(\tau))\delta(\mathbf{u}^2-1)\exp\left\{-\frac{1}{2}\kappa\int_0^N d\tau\left[\frac{d\mathbf{u}}{d\tau}\right]^2 + i\frac{\theta}{2\pi}\int_0^N d\tau\frac{d}{d\tau}\tan^{-1}\left[\frac{u^y}{u^x}\right]\right\}$$
$$\times\exp\left\{ i\mathbf{p}\cdot\int_0^N \mathbf{u}(\tau)d\tau\right\}, \tag{4.12b}$$

where the normalization $\mathfrak{J}$ is chosen in such a way that for $\mathbf{p}=0$ we have $\langle\ \rangle=1$. Using Eq. (4.12) and results of Polyakov [20], let us consider the following expansion:

$$\left\langle \exp\left[i\mathbf{p}\cdot\int_0^N \mathbf{u}\right]\right\rangle = 1 - i\mathbf{p}\cdot\int_0^N\langle\mathbf{u}(\tau)\rangle d\tau - p_\alpha p_\beta\int_0^N d\tau\int_0^\tau d\tau'\langle u_\alpha(\tau)u_\beta(\tau')\rangle + \cdots , \tag{4.13}$$

where α,β are the Cartesian coordinates. By symmetry, the first term vanishes while for the second term we have

$$\langle u_\alpha(\tau)u_\beta(\tau')\rangle = \sum_{l\neq 0}\langle 0|u_\alpha|l\rangle\langle l|u_\beta|0\rangle e^{-(E_l-E_0)|\tau-\tau'|\kappa} . \tag{4.14}$$

The right-hand side of Eq. (4.14) was explicitly calculated in [49] [e.g., see Eq. (2.14) of this reference] so that we have (for $0\le\theta\le\tau$)

$$\langle u_\alpha(\tau)u_\beta(\tau')\rangle = \delta_{\alpha\beta}\sum_{l\neq 0}\frac{1}{l^2}\exp\left[-\frac{\kappa}{2}l\left[l-\frac{\theta}{\pi}\right]|\tau-\tau'|\right] . \tag{4.15}$$

For $\theta=\pm\pi$ and $l=\pm 1$ the term in the exponent vanishes and, for $|\tau-\tau'|\to\infty$ it becomes the leading term in the expansion of the correlator. Using this fact in Eq. (4.13) produces

$$\left\langle \exp\left[i\mathbf{p}\cdot\int_0^N \mathbf{u}\right]\right\rangle = 1-\frac{\mathbf{p}^2}{2}N^2+O(\mathbf{p}^4) . \tag{4.16}$$

The same result can be obtained following Polyakov's ingenuous trick [50] (which was later on proven rigorously in [51]). The trick lies in the fact that, instead of u averaging defined in Eq. (4.12), one can perform spin averaging by using properties of Pauli matrices σ_i (e.g., compare with Sec. II):

$$\mathrm{Tr}\sigma_i=0 \quad\text{but}\quad \mathrm{Tr}\sigma_i^2=1 . \tag{4.17}$$

If we formally write

$$\left\langle \exp\left[i\mathbf{p}\cdot\int_0^N \mathbf{u}\right]\right\rangle \equiv \langle \exp i\mathbf{p}\cdot\boldsymbol{\sigma}N\rangle_\sigma , \tag{4.18}$$

then, when the right-hand side of Eq. (4.18) is expanded and the traces over σ_i's are taken, the result, Eq. (4.16), is recovered. Equation (4.18) is proven rigorously in [51] and is based on the observation that the Seret-Frenet equations for the moving frame along the curve have the same mathematical structure as equations of motion for the precessing spin (as it was already noticed and used in our earlier work [37]).

Laplace transforming the right-hand side of Eq. (4.18) produces

$$\int_0^\infty e^{-sN}\langle \exp i\mathbf{p}\cdot\boldsymbol{\sigma}N\rangle_\sigma = \left\langle\frac{1}{i\mathbf{p}\cdot\boldsymbol{\sigma}-s}\right\rangle_\sigma , \tag{4.19}$$

which has to be compared with Eq. (2.6). Obviously, Eq. (4.19) describes the Dirac propagator in $d=2$.

The above analogy with the Dirac propagator exists, however, only for a special value of θ: $\theta=\pi$. For $\theta\neq\pi$ the analogy is lost, but the relevant physical results such as Eq. (4.15) are not much affected. Indeed, if we were interested in calculating $\langle\mathbf{R}^2\rangle$, then using Eq. (4.15) and keeping only the $|l|=1$ term the ground state dominance, which is permissible in the limit $|\tau-\tau'|\to\infty$, we obtain

$$\langle u_\alpha(\tau)u_\beta(0)\rangle \cong \delta_{\alpha\beta}2\exp\left[-\frac{1}{2}\kappa\tau\right]\cosh\left[\frac{1}{2}\frac{\kappa\theta\tau}{\pi}\right] , \tag{4.20}$$

which coincides with Eq. (4.5) of [49], as expected. The $\langle\mathbf{R}^2\rangle$ can now be obtained in a standard way (e.g., see [52]):

$$\langle\mathbf{R}^2\rangle = \int_0^N d\tau\int_0^N d\tau' 2\exp\left[-\kappa\frac{|\tau-\tau'|}{2}\right]$$
$$\times\cosh\left[\kappa\frac{\theta}{2\pi}|\tau-\tau'|\right]$$
$$=2a_1^2\rho(x_1)+2a_2^2\rho(x_2) , \tag{4.21}$$

where

$$a_1=\frac{2}{(1-\theta/\pi)},\quad x_1=\frac{\kappa N}{a_1},\quad a_2=\frac{2}{(1+\theta/\pi)},\quad x_2=\frac{N\kappa}{a_2} ,$$
$$\rho(x)=x-1+\exp(-x) . \tag{4.22}$$

Let us consider now two limiting cases: $\theta\to 0$ and $\theta\to\pi$. For $\theta=0$ we obtain $a_1=a_2$ and $x_1=x_2$. From this we retrieve the standard Kratky-Porod (KP) result. Let now $\theta\to\pi^-$ and $N\to\infty$ but $eN\ll 1$ where $e=1-\theta/\pi$. Using Eq. (4.21) we obtain

$$\langle\mathbf{R}^2\rangle = 2\left[\frac{2}{e}\right]^2\left[\frac{N}{2}e-1+1-\frac{N}{2}e+\frac{1}{2}\left[\frac{N}{2}e\right]^2+\cdots\right]$$
$$+2[N-1+\exp(-N)]\to N^2 . \tag{4.23}$$

From this, the parameter θ is effectively responsible for the rigidity of the chain. This can be accomplished as well by the use of the Dirac propagator, employing Eqs. (2.5), (2.6), and (4.19), if the proper identification is made. For instance, if we identify *is* in Eq. (4.19) with *im* [e.g., see Eq. (2.6)] and take into account that the Laplace variable in particle physics is always treated as the mass [12] and, in addition, we identify one of the p components with the variable conjugate to "time" (polymer length). This can be achieved either by restricting one of the p's to $p>0$ or by adding a small $\pm i\varepsilon$ term to the mass to assure that the corresponding Green's function is retarded (as it is always done in field-theoretic calculations [36]). Therefore Eq. (4.12b) acts effectively as a Dirac propagator for $0\leq\theta\leq\pi$ and becomes strictly Dirac in the limit $\theta=\pi$. For $\theta\neq 0,\pi$ Eq. (4.21) does not provide the KP result for $\langle \mathbf{R}^2\rangle$ whereas Eq. (2.5) *does* recover this limit as demonstrated in [11]. The deviations from KP are naturally negligible in the limit $N\to\infty$. Finally, even for $\theta=0$ the result given by Eq. (4.23) can be obtained. In this case for $1/\kappa\to 0$ we would obtain the result given by Eq. (4.23). Formally, we can regulate the rigidity either by changing κ for fixed θ or by changing θ for fixed κ (of course, we also can change both θ and κ at the same time). In the literature it is common to associate the Dirac propagator with the case when $1/\kappa\to\infty$ (e.g., see [20]), whence the rigidity effects in this traditional case are being regulated by θ. Equation (4.20) deserves also a discussion with respect to renormalization of bending rigidity. Rewriting the cosh in Eq. (4.20) in terms of two exponential functions it is seen that the stiffness becomes renormalized, i.e.,

$$\langle u_\alpha(\tau)u_\beta(0)\rangle \propto \delta_{\alpha\beta}\exp\left\{-\frac{1}{2}\kappa\left[1\pm\frac{\theta}{\pi}\right]\tau\right\} . \quad (4.24)$$

In view of Eq. (4.23), the other term is not important for $N\to\infty$. Therefore the chain has become effectively stiffer by the presence of the θ term, i.e., $\kappa_R=\kappa(1+\theta/\pi)$.

V. SCHRÖDINGER-LIKE EQUATION ANALYSIS OF THE NONLINEAR σ MODEL IN EXTERNAL FIELDS

In the preceding section we have introduced the Hamiltonian for the planar rotator $\hat{H}_\phi$ given by Eq. (4.6). Consider now the stationary Schrödinger-like equation for the Hamiltonian $\hat{H}_\phi$ in the presence of the nematic and the elongation fields. In this case we obtain

$$\left[-\frac{1}{2}\kappa\frac{d^2}{dx^2}+g\cos^2 x+f\cos x\right]\psi=E\psi , \quad (5.1)$$

where $0\leq x\leq\pi$ and $x=\phi$, e.g., see Eq. (4.6).

Use of Eq. (4.10) produces instead

$$\left[-\frac{1}{2}\kappa\frac{d^2}{dx^2}+\frac{1}{2}\kappa\frac{i\theta}{\pi}\frac{d}{dx}+\frac{1}{2}\kappa\left[\frac{\theta}{2\pi}\right]^2 +g\cos^2 x+f\cos x\right]\psi=E\psi . \quad (5.2)$$

Using the fact that $\cos^2 x=\frac{1}{2}(\cos 2x+1)$, Eq. (5.1) can be brought into the standard form of the Whittaker-Hill equation [25] while for $f=0$ we have the case of the Mathieu equation [26]. Following [52] and using substitution (for simplicity, we set $\kappa=2$)

$$\psi=w(x)\exp\left[-\frac{i\theta}{2\pi}x\right] \quad (5.3)$$

in Eq. (5.2) removes the unwanted θ terms and brings Eq. (5.2) back to the form of Eq. (5.1). These results need to be compared with that discussed in Sec. IV.

Consider now the three-dimensional Schrödinger-like equation discussed in [15] by WGB [e.g., see Eq. (4.5) of [15]]. Writing in this equation $\Lambda_n+\Delta^2=-E$ we obtain

$$\left[\frac{d^2}{dx^2}+\cot x\frac{d}{dx}-g\cos^2 x\right]\psi=E\psi , \quad (5.4)$$

where we used x instead of θ and g instead of Δ^2 used in this reference.

We would like now to demonstrate that Eqs. (5.1) and (5.4) are mathematically closely related [of course, we have to set $f=0$ in Eq. (5.1) or to add the corresponding term in Eq. (5.4)]. To do so, following [53] consider the substitution $\psi=z(x)\sqrt{\sin x}$ in Eq. (5.1). This produces

$$\left[\frac{d^2}{dx^2}+\cot x\frac{d}{dx}-g\cos^2 x-\frac{1}{4}-\frac{1}{4\sin^2 x}\right]z(x)=Ez(x) . \quad (5.5)$$

This equation is different from Eq. (5.4). However, it is a physically correct equation which is related to the Dirac monopole (see next section); Eq. (5.5) is also known as the associated Mathieu equation and is a special case of a spheroidal wave equation [54]. It should be noted, however, that the spheroidal Eq. (5.5) is *not the same as Eq. (4.3) of [15] which the authors also call "spheroidal."* Moreover, Eq. (5.4), is *not* the same as the Schrödinger-like equation for a double well discussed in Sec. II in connection with the 1D Ising model describing hairpins. On the other hand, Eq. (5.1), *is* for small x the desired double well equation for the hairpins. Indeed, expanding cosine terms in (5.1) we obtain approximately

$$\left[-\frac{1}{2}\kappa\frac{d^2}{dx^2}-a_1x^2+a_2x^4\right]\psi=\tilde{E}\psi , \quad (5.6)$$

where $a_1=g+f/2$, $a_2=\frac{1}{12}a_1$. Therefore Eq. (5.6) reduces to the double well equation under conditions where this expansion is appropriate. Formally, Eq. (5.6) provides the answers to questions posed in Sec. II. Expansion of cosine terms is not too illuminating, however, in the light of a wide literature discussing Mathieu and Whittaker-Hill equations. For illustrative purposes, we shall confine ourselves (only in this section) to the qualitative discussion related to the Mathieu equation, i.e., Eq. (5.1) with $f=0$. This equation is known in physical literature [29] in connection with problems which involve chaos. This is not accidental in view of the analysis of the *XXZ* model presented in [41]. The physical picture can be described as follows. Let the coefficients a_1 and a_2

be initially zero. Then the eigenfunctions given by Eq. (4.8) (for $\kappa=2$) are the correct unperturbed eigenfunctions. Now let a_1 and a_2 (or more generally g) be nonzero. In this case, the eigenvalues and eigenfunctions get perturbed. Among the perturbations only those are admissible which *do not* violate the condition given in Eq. (4.7). This leads to the conclusion that *not* all values of the parameter g (and also f if it is nonzero) are permissible. *The system will not respond to perturbations from the forbidden region of values for g.* In cases (other than ours) when the values of g from the forbidden region are used, the chaotic behavior is observed.

Let us make the above arguments more precise. Following the mathematical literature on these classical equations [30,53], we rewrite Eq. (5.1) in the standard form:

$$\frac{d^2}{dx^2}\psi+[\delta-2\varepsilon\cos 2x]\psi=0\ , \tag{5.7}$$

where $\delta=(2/\kappa)(-g+E)$, $2\varepsilon=(1/\kappa)g$, and the function ψ is subject to the boundary conditions given by Eq. (4.7). In view of [15], some minor rearrangements were made to arrive at (5.7). For instance, because of Eq. (3.9) and taking into account that we are studying a two-dimensional planar problem first, the factor of 3 in Eq. (3.9) is replaced by factor of 2, etc.

Since Eq. (5.7) is a second order differential equation, we expect that it has two solutions. Let ψ_1 and ψ_2 be its solutions. Then, both of them should satisfy Eq. (4.7). However, if we change $x\to x+\pi$, Eq. (5.7) is obviously unchanged. Thus among solutions of Eq. (5.7) there should be those possessing period π. Evidently, such solutions will have a period of 2π and, whence, could be made to satisfy Eq. (4.7). The wave function, Eq. (4.7), already has a standard Floquet form [30,55] which is used in the theory of Mathieu and Hill equations, i.e.,

$$\psi(x)=\exp\left[i\frac{\theta}{2\pi}x\right]\Phi(x)\ , \tag{5.8}$$

where the function Φ is periodic with natural period 2π. Obviously, two major periods are of importance: π (caused by perturbation) and 2π (natural frequency) and therefore we should expect a situation similar to that encountered in the theory of commensurate-incommensurate (C-I) transitions [23,24]. Indeed, in view of Eq. (4.11), the classical action can be written as

$$S=\int_0^{2\pi}dt\left[\frac{\kappa}{2}\left[\frac{d\phi}{d\tau}-\delta\right]^2+V(\tau)\right]\ , \tag{5.9}$$

where $V(\tau)$ is the periodic function of τ, e.g., $\cos 2\tau$, and δ is equal to $\theta/4\pi$. We just demonstrated therefore that the underlying physics of the hairpin problem is exactly the same as in the theory of C-I transitions for which an enormous literature exists [24]. This is not too surprising in view of the fact that both problems stem from study of the same XXZ model [23] and admit the same fermionic (exact) and approximate bosonic quantum many-body treatments (see, for example, [56] for bosonic treatment). The analogy with C-I transition is formally lost when the three-dimensional case is considered but, in view of Eqs. (5.1) and (5.5), we still can use the Schrödinger-like equation of the type given by Eq. (5.7). Because of this, it is worthwhile to investigate this equation based on results known in the mathematical literature.

In the spirit of the Floquet theory [30,55] let us write $\theta/2\pi=\beta^{(0)}$. Evidently, the perturbations caused by the nonzero g will change $\beta^{(0)}$, i.e., we anticipate $\beta=\beta(g)$ and $\beta(g=0)=\beta^{(0)}$, whence, in complete agreement with general analysis of Secs. II and IV, the presence of nematic interactions is expected to lead to the renormalization of the rigidity parameters so that knowledge of the explicit form of $\beta(g)$ provides the answers to the questions posed in Sec. II.

For simplicity, let us fix the initial rigidity parameter, $\kappa=2$, and let

$$\psi_{1,2}=\exp(\pm i\beta x)\Phi_{1,2}(x)\ . \tag{5.10}$$

Substitution of Eq. (5.19) into (5.1) produces

$$\frac{d^2}{dx^2}\Phi_{1,2}\pm 2i\beta\frac{d}{dx}\Phi_{1,2}+(\delta-\beta^2-2\varepsilon\cos 2x)\Phi_{1,2}=0\ . \tag{5.11}$$

For small g we look for perturbative solutions of Eq. (5.11) of the form

$$\begin{aligned}&\Phi_{1,2}(x,\varepsilon)=\Phi^{(0)}(x)+\varepsilon\Phi^{(1)}(x)+\cdots\ ,\\&\delta(x,\varepsilon)=\delta^{(0)}+\varepsilon\delta^{(1)}+\cdots\ ,\\&\beta(x,\varepsilon)=\beta^{(0)}+\varepsilon\beta^{(1)}+\cdots\ .\end{aligned} \tag{5.12}$$

Substitution of Eq. (5.12) into Eq. (5.11) produces

$$\frac{d^2}{dx^2}(\Phi^0+\varepsilon\Phi^{(1)}+\cdots)\pm 2i(\beta^{(0)}+\varepsilon\beta^{(1)}+\cdots)\frac{d}{dx}(\Phi^{(0)}+\varepsilon\Phi^{(1)}+\cdots)$$
$$+[\delta^{(0)}+\varepsilon\delta^{(1)}-(\beta^{(0)}+\varepsilon\beta^{(1)}+\cdots)^2-2\varepsilon\cos 2x](\Phi^{(0)}+\varepsilon\Phi^{(1)}+\cdots)=0\ . \tag{5.13}$$

Collecting terms we obtain

$$\varepsilon^0:\ \frac{d^2}{dx^2}\Phi^{(0)}\pm 2i\beta^{(0)}\frac{d}{dx}\Phi^{(0)}+[\delta^{(0)}-(\beta^{(0)})^2]\Phi^{(0)}=0\ , \tag{5.14}$$

$$\varepsilon^1:\ \frac{d^2}{dx^2}\Phi^{(1)}\pm 2i\beta^{(0)}\frac{d}{dx}\Phi^{(1)}+[\delta^{(0)}-(\beta^{(0)})^2]\Phi^{(1)}=\pm 2i\beta^{(1)}\frac{d}{dx}\Phi^{(0)}-\delta^{(1)}\Phi^{(0)}+2\beta^{(0)}\beta^{(1)}\Phi^{(0)}+2\Phi^{(0)}\cos 2x\ . \tag{5.15}$$

The solution of Eq. (5.14) produces again Eq. (4.8) as required. In order to use Eq. (4.8) in Eq. (5.15) it is useful to notice that solution $\Phi^{(0)}$ can be formally written as

$$\Phi_l^{(0)} = a\cos lx + b\sin lx \ , \tag{5.16}$$

where at the end of the calculations one can set $a=b$ and determine a by normalization condition as usual. Notice that *both* $\cos lx$ and $\sin lx$ would fit Eqs. (4.7) and (5.8), (5.10). If we use Eq. (5.16) in the right-hand side of Eq. (5.15), then, for example, for $l=1$ we obtain for this equation the following result:

$$\varepsilon^1: \ \frac{d^2}{dx^2}\Phi^{(1)} \pm 2i\beta^{(0)}\frac{d}{dx}\Phi^{(1)} + [\delta^{(0)} - (\beta^{(0)})^2]\Phi^{(1)} = \pm 2i\beta^{(1)}(-a\sin x + b\cos x) - (\delta^{(1)} - 2\beta^{(0)}\beta^{(1)})(a\cos x + b\sin x) + 2(a\cos x + b\sin x)\cos 2x \ . \tag{5.17}$$

Using the trigonometric relations,

$$\cos x\cos 2x = \tfrac{1}{2}[\cos 3x + \cos x] \ ,$$
$$\sin x\cos 2x = \tfrac{1}{2}[\sin 3x - \sin x] \ ,$$

and requiring the secular (i.e., proportional to $\sin x$ and $\cos x$) terms to vanish [30], we obtain the following system of equations:

$$\begin{aligned} &\pm 2i\beta^{(1)}a - (\delta^{(1)} - 2\beta^{(0)}\beta^{(1)} + 1)b = 0 \ , \\ &-(\delta^{(1)} - 2\beta^{(0)}\beta^{(1)} - 1)a \pm 2i\beta^{(1)}b = 0 \ . \end{aligned} \tag{5.18}$$

By requiring the determinant of the above system of equations to vanish, we then obtain

$$4(\beta^{(1)})^2 - [(\delta^{(1)} - 2\beta^{(0)}\beta^{(1)})^2 - 1] = 0 \ . \tag{5.19}$$

The consistency check requires us to set $\beta^{(0)}=0$ first. This then implies

$$\beta^{(1)} = \pm\tfrac{1}{2}\sqrt{(\delta^{(1)})^2 - 1} \tag{5.20}$$

in complete accord with [30] [see Eq. (11.107) of Ref. [30]]. Equation (5.20) is very interesting because it requires $\delta^{(1)} \geq 1$ in order for Eq. (4.7) to hold. To put this in another form is to say that β is *not allowed* to acquire an imaginary part. In the theory of dynamical systems such an imaginary part yields an instability and leads to chaos [29]. In our case, using Eqs. (5.7) and (5.12) we obtain effectively

$$\delta^{(1)} = \hat{\delta}^{(1)} - 2 \ , \tag{5.21}$$

where, again in complete agreement with [30], the factor $\hat{\delta}^{(1)}$ is left undetermined (i.e., it can vary without restrictions in the physically allowed domain to be discussed below). Using Eq. (5.21) in (5.20) we have to require

$$(\hat{\delta}^{(1)})^2 - 4\hat{\delta}^{(1)} + 3 \geq 0 \ . \tag{5.22}$$

This produces $0 \leq \hat{\delta}^{(1)} \leq 1$ and $\hat{\delta}^{(1)} \geq 3$ and, accordingly, using Eq. (5.12), the transition curves emanating from $\delta=1$ are

$$\delta = 1 \pm \varepsilon + O(\varepsilon^2) \ . \tag{5.23}$$

This result is in complete agreement with that obtained in [30], as required. Now let $\beta^{(0)} \neq 0$, then using Eq. (5.19) we obtain

$$(\beta^{(1)})^2 + \frac{\delta^{(1)}\beta^{(0)}}{1-(\beta^{(0)})^2}\beta^{(1)} + \frac{1-(\delta^{(1)})^2}{4[1-(\beta^{(0)})^2]} = 0 \ . \tag{5.24}$$

Noticing that, by construction $\beta^{(0)} < 1$, we obtain

$$\beta^{(1)}_{1,2} = \frac{\beta^{(0)}}{2[1-(\beta^{(0)})^2]}\left[-1 \pm \left\{1 - \frac{1}{(\beta^{(0)})^2}[1-(\delta^{(1)})^2] \times [1-(\beta^{(0)})]^2\right\}^{1/2}\right] . \tag{5.25}$$

Because $\beta^{(0)} < 1$ and $\delta^{(1)} > 1$, by construction, the result for $\beta^{(1)}$ is real and therefore makes physical sense.

Let us make some qualitative remarks on some elementary physical applications of the results obtained so far. To this purpose let us analyze the behavior of the correlation function defined by Eq. (4.15) in the absence of perturbations.

Taking into account Eq. (4.9) and rewriting it in notations used in this section we obtain

$$E_l = \tfrac{1}{2}(\sqrt{\delta_l} - \beta_l)^2 \ . \tag{5.26}$$

We have supplied δ and β with subscript l because the above quantities are actually l dependent as can be seen from the deviation given above. Evidently, we have

$$\begin{aligned} \delta_l &= l^2 + \varepsilon\delta_l^{(1)} + \varepsilon^2\delta_l^{(2)} + \cdots \ , \\ \beta_l &= \beta^{(0)} + \varepsilon\beta_l^{(1)} + \varepsilon^2\beta_l^{(2)} + \cdots \ , \end{aligned} \tag{5.27}$$

where $\beta^{(0)} = \theta/2\pi$. Consider now the difference between 1 and the ground state $E_1 - E_0$ with accuracy up to $O(\varepsilon')$:

$$E_1 - E_0 = \tfrac{1}{2}[1 - 2\beta^{(0)} + 2\varepsilon f(\delta_1^{(1)}, \beta_1^{(1)}, \beta_0^{(0)}, \delta_0^{(2)})] \ , \tag{5.28}$$

where $f(\delta_1^{(1)}, \beta_1^{(1)}, \beta_0^{(0)}, \delta_0^{(2)})$ is a linear combination of the above coefficients (we have taken into account here that $\delta_0^{(1)} = 0$ [30]). Using the results of Sec. IV, we know that for $2\beta^{(0)} = 1$ the polymer chain is fully stretched and behaves as a rigid rod. Now, under the action of perturbation, several things could happen: first, if $2\beta^{(0)}$ was initially less than 1, then the perturbation can bring it to 1, in principle. In view of Eq. (5.23), this process may be discontinuous because both $\delta_1^{(1)}$ and $\beta_1^{(1)}$, as well as $\delta_0^{(2)}$ have branches so that when g increases (decreases) one expects to observe a conformational jump which can be interpreted as hairpin destruction (creation). [The above process is also related to the nematic-(stretch) isotropic (coil) phase transition [57].] In the last case one usually studies the behavior of E_0 related to the free energy of the system [57]. We plan to give a detailed treatment of these processes in future publications while here we would like to provide an additional physical application of the obtained results. To this purpose, let us consider once again Whittaker-Hill (WH) Eq. (5.1). For $f\neq 0$, following [27], let us rewrite Eq. (5.1) by rescaling the variable x to $2x$ in the form

$$\frac{d^2}{dx^2}\psi+[\lambda+4mq\cos 2x+2q^2\cos 4x]\psi=0\ , \qquad (5.29)$$

where $\lambda=4\delta$, $2q^2=-8\varepsilon$, $4mq=-4f$, and m is so far an arbitrary real number. From the theory of WH equations [27] it is known that (a) in order for the periodic solution to exist, $2q^2$ must be non-negative and (b) it is possible to have two linearly independent periodic solutions, if, and only if, m is an integer. The first requirement forces us to change ε into $-\varepsilon$ in Eq. (5.29) and then also in the rest of our calculations. We have checked that up to $O(\varepsilon^1)$ this causes no change in our results. The higher order (in ε) terms are different (in general) [25,30]. It is important to realize that this requirement to change ε into $-\varepsilon$ is possible to detect *only* if an extra f term is considered. Because the authors of [15] have not included the f term, our treatment presented above faithfully followed their initial assumptions. The fact that m must be an integer is also rather remarkable because it tells us that the external (non-nematic) stretching force *should be quantized.* There is *no* such requirement in the absence of a nematic matrix as we have demonstrated before [1].

Further studies [25] have shown that if the $2q^2$ term in Eq. (5.29) is negative, then it is also possible to obtain periodic solutions. For such solutions the non-nematic force is not discrete and these solutions are quite different from those which correspond to the case when $2q^2$ is positive. Physically, the first case seems to be more acceptable because the discreteness of force can be attributed to the discreteness of the hairpin energies, i.e., by stretching the polymer chain the hairpins are destroyed one by one. Whether or not this is correct can only be resolved experimentally. We hope that such experiments will be performed in the future.

This concludes our qualitative treatment of the two-dimensional case. It is of interest now to see to what extent the results obtained so far could be preserved in three-dimensions. This is a topic of the next section.

VI. NONLINEAR σ MODEL IN THREE-DIMENSIONS AND THE DIRAC MONOPOLE

In the preceding section we have obtained Eq. (5.5) from Eq. (5.1) by the appropriate change of variables. *The presence of a term $\sim 1/\sin^2 x$ is crucial in bringing Eq. (5.5) into the form of Eq. (5.1), which admits a double well interpretation.* In the treatments existing in the literature this term is completely ignored. Here we would like to emphasize that *the presence of this term is motivated by much deeper reasons than just reduction of Eq. (5.5) to Eq. (5.1).* Its origin can be traced to the Wess-Zumino term [19,20], Eq. (4.4), which must be present in three-dimensional path integral Eq. (4.3) due to nonzero torsion for three-dimensional curves as it was explained in [37] and Sec. IV.

In complete analogy with Eq. (4.12), we introduce the generating function (in three dimensions)

$$\left\langle \exp\left[i\mathbf{p}\cdot\int_0^N \mathbf{u}(\tau)d\tau\right]\right\rangle=\Im\int_{\mathbf{u}_i=\mathbf{u}_f} D(\mathbf{u}(\tau))\delta(\mathbf{u}^2-1)\exp\left\{-\frac{1}{2}\kappa\int_0^N d\tau\left[\frac{d\mathbf{u}}{d\tau}\right]^2+i\Theta\int_0^N d\tau\, C(\mathbf{u}(\tau))\right\}$$
$$\times\exp\left\{i\mathbf{p}\cdot\int_0^N \mathbf{u}(\tau)d\tau\right\}, \qquad (6.1)$$

where $C(\mathbf{u}(\tau))$ is defined by Eq. (4.5) and, as before, the normalization factor $\Im$ is again chosen such that $\langle\ \rangle=1$ for $\mathbf{p}=\mathbf{0}$.

Although there is a large amount of literature on path integrals given by Eq. (6.1), for our purposes we shall select only those papers that are directly connected with the results presented in Sec. IV. The earliest observation that the path is integral, (6.1), with $\mathbf{p}=\mathbf{0}$, is related to the Dirac magnetic monopole that was made in [54]. In [31] this treatment was somewhat refined while further details of this refinement appeared in [48]. Because of the existing literature, we provide only an outline of results needed for the reading of the rest of our paper.

Begin with the observation that the tangent vector $\mathbf{u}$ can be presented in the form [12,48]

$$\mathbf{u}=(\mathbf{z}^\dagger\sigma\mathbf{z})\ , \qquad (6.2)$$

where $\mathbf{z}$ is two-dimensional complex vector $\mathbf{z}=(z_1,z_2)$ which is normalized to unity and σ, as before, Pauli matrices. Because $(\sigma_i)^2=1$ we then obtain

$$\mathbf{u}^2=|z_1|^2+|z_2|^2=1 \qquad (6.3)$$

as required. Furthermore, if $z_1=x_1+ix_2$ and $z_2=x_3+ix_4$, then

$$u_1=(x_1-ix_2,x_3-ix_4)\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}x_1+ix_2\\x_3+ix_4\end{bmatrix}$$
$$=2(x_1x_3+x_2x_4)\ , \qquad (6.4)$$

analogously,

$$u_2=2(x_1x_4-x_2x_3)\ , \qquad (6.5)$$

$$u_3=x_1^2+x_2^3-x_3^2-x_4^2\ , \qquad (6.6)$$

and, from Eq. (6.3), we also have

$$x_1^2+x_2^2+x_3^2+x_4^2=1\ . \tag{6.7}$$

If now

$$z_1=e^{i\chi}\cos\theta/2,\quad z_2=e^{i(\varphi+\chi)}\sin\theta/2\ , \tag{6.8}$$

then a little algebra produces straightforwardly

$$\begin{aligned} u_1&=\sin\theta\cos\varphi\ ,\\ u_2&=\sin\theta\sin\varphi\ ,\\ u_3&=\cos\theta\ . \end{aligned} \tag{6.9}$$

With such parametrization, let us consider the term $(d\mathbf{u}/d\tau)^2$ in the exponent of Eq. (6.1). It is shown in [48] that

$$\tfrac{1}{2}\dot{\mathbf{u}}^2=2\dot{\mathbf{z}}^\dagger\dot{\mathbf{z}}-2a^2\ , \tag{6.10}$$

where

$$a=i\mathbf{z}^\dagger\dot{\mathbf{z}} \tag{6.11}$$

and the dot denotes the derivative with respect to the parametrization $d/d\tau$, as usual. For $\mathbf{p}=\mathbf{0}$ the action in the exponent of (6.1) can be written as

$$S=\int_0^N d\tau[2\kappa\{(\dot{\mathbf{z}}^\dagger\dot{\mathbf{z}})-a^2\}-2\Theta a]\ , \tag{6.12}$$

where $2\Theta=0,\pm1,\pm2$. Notice that unlike the two-dimensional case, Θ *must* be quantized in three dimensions. Introduce now the matrix $\mathbf{s}$ via

$$\mathbf{s}=\begin{bmatrix} e^{i(\alpha+\gamma)/2}\cos\beta/2 & e^{i(\gamma-\alpha)/2}\sin\beta/2\\ -e^{-i(\gamma-\alpha)/2}\sin\beta/2 & e^{-i(\alpha+\gamma)/2}\cos\beta/2\end{bmatrix}, \tag{6.13}$$

where α,β,γ are Euler's angles. It can be shown that

$$\mathrm{tr}(\dot{\mathbf{s}}^\dagger\dot{\mathbf{s}})=2\dot{\mathbf{z}}^\dagger\dot{\mathbf{z}} \tag{6.14}$$

and

$$a=\tfrac{1}{2}\mathrm{tr}(\sigma_3\mathbf{s}^{-1}\dot{\mathbf{s}})\ . \tag{6.15}$$

Because of these relations, it is possible to write

$$\mathrm{tr}(\dot{\mathbf{s}}^\dagger\dot{\mathbf{s}})=\tfrac{1}{2}\dot\beta^2+\tfrac{1}{2}(\dot\gamma+\dot\alpha\cos\beta)^2+\tfrac{1}{2}\dot\alpha^2\sin^2\beta\ . \tag{6.16}$$

Note that this expression coincides exactly with that for the kinetic energy of a symmetric top [e.g., see Ref. [58], Eq. (4.8.3), where one has to set the inertia moments $I_1=I_3$]. By combining Eqs. (6.12)–(6.15) it is possible to show that the Lagrangian for the action, Eq. (6.12), is that for the three-dimensional symmetric top but with the square of the third angular component being subtracted. Quantization of such a Lagrangian then proceeds in a usual way, i.e., through the Hamiltonian formalism.

To illustrate the above ideas, consider the Schrödinger equation for the fully symmetric top [58] first. We obtain

$$\left[\frac{\partial^2}{\partial\beta^2}+\cot\frac{\partial}{\partial\beta}+\frac{1}{\sin\beta}\left[\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial\gamma^2}-2\cos\beta\frac{\partial^2}{\partial\alpha\partial\gamma}\right]+l(l+1)\right]D_{mk}^{(l)}(\alpha,\beta,\gamma)=0\ , \tag{6.17}$$

where functions $D_{mk}^{(l)}(a,b,g)$ are the usual Wigner D functions defined by

$$D_{mk}^{(l)}(\alpha,\beta,\gamma)=\exp(im\alpha)d_{mk}^{(l)}(\beta)\exp(ik\gamma)\ . \tag{6.18}$$

Substitution of Eq. (6.18) into Eq. (6.17) produces

$$\left[\frac{d^2}{d\beta^2}+\cot\beta\frac{d}{d\beta}-\frac{m^2+k^2-2mk\cos\beta}{\sin^2\beta}+l(l+1)\right]\times d_{mk}^{(l)}(\beta)=0\ . \tag{6.19}$$

Finally, let us write $k^2=k^2\cos^2\beta+k^2\sin^2\beta$. This produces

$$\left[-\frac{d}{d\beta^2}-\cot\beta\frac{d}{d\beta}+\frac{(m-k\cos\beta)^2}{\sin^2\beta}\right]d_{mk}^{(l)}(\beta)=[l((l+1)-k^2]d_{mk}^{(l)}(\beta)\ . \tag{6.20}$$

Equation (6.20) coincides exactly with Eq. (2.2) of Wu and Yang [59] for the magnetic Dirac monopole. In view of this result, and taking into account Ref. [60], we reach the following conclusions. First, the presence of the Θ term in Eq. (6.1) is responsible for k subtraction in the right-hand side of Eq. (6.20). Second, the parameter Θ is associated with k, i.e., $\Theta=k$. Third, k and l can have integer or half-integer values. The smallest half-integer value of k is $\pm(\frac{1}{2})$. For this case it is known [58] that $d_{1/2\,1/2}^{(1/2)}(\beta)=d_{-1/2-1/2}^{(1/2)}(\beta)=\cos\beta/2$, i.e., there is a degeneracy. In analogy with Eq. (4.13), we expand the p exponent in Eq. (6.1), then, because of this degeneracy, in the limit $|\tau-\tau'|\to\infty$ we will end up with the same result, Eq. (4.16), and Eqs. (4.18), (4.19) follow [20]. An alternative proof can also be found in [51]. Notice, if k were ±1, we would also have a degeneracy, e.g., $d_{11}^{(1)}(\beta)=d_{-1-1}^{(1)}(\beta)=\frac{1}{2}(1+\cos\beta)$. But this time there is also another intermediate state with $k=0$ and therefore the arguments leading to Eq. (4.16) would not be applicable. At the same time, the result of the type of Eq. (4.19) would still hold, e.g., see [51]. For k values *other* than $\pm\frac{1}{2}$ we obtain [using Eq. (6.1)] propagators for particles with higher spins. Our experience with the two-dimensional case (even though limited because θ is *not* quantized) suggests that these higher order spin propagators may be responsible for the stiffening of the chain. This is also important for the development of the topological theory of reputation as indicated in our earlier work [21,61].

Now let $m=\frac{1}{2}=k$ in Eq. (6.20) (i.e., Dirac equation case); we obtain

$$\left[-\frac{d^2}{d\beta^2}-\cot\beta\frac{d}{d\beta}+\frac{1}{4}\tan^2\frac{\beta}{2}\right]d_{1/2\,1/2}^{(1/2)}(\beta)=Ed_{1/2\,1/2}^{(1/2)}(\beta)\ . \tag{6.21}$$

Historically, this equation was obtained by Dirac himself [e.g., see his Eq. (13) of Ref. [62]]. Moreover, given that Eq. (6.20) originates from Eq. (6.17), it is possible, following [63] to redefine the angle γ in such a way that the resulting (6.21) will acquire the form

$$\left[-\frac{d^2}{d\beta^2}-\cot\beta\frac{d}{d\beta}+\frac{1}{4}\cot^2\beta\right]d^{(1/2)}_{1/2\,1/2}(\beta)$$
$$=Ed^{(1/2)}_{1/2\,1/2}(\beta)\ , \quad (6.22)$$

which, incidentally, coincides exactly with that used in [64] [e.g., see Eq. (29) of [64]]. *Obviously, Eq. (6.22) can be reduced to Eq. (5.5)* (for $g=0$) *and, therefore, the connection with the Dirac equation is established.* Therefore the double well potential picture of hairpins proposed by de Gennes [6] and developed by others is *directly connected with the Dirac equation and Dirac monopole.*

VII. BEYOND THE DIRAC MONOPOLE

The results presented in Sec. V involve perturbative methods which require the nematic coupling constant g to be small. If this is not the case, other methods should be used. Here we would like to provide only an introduction to these methods, leaving detailed calculations for further study.

Following Mozer [65], let us consider first the classical motion of a "particle" constrained to the sphere. The action ($\kappa=1$) for this case is given by

$$S=\frac{1}{2}\int_0^N d\tau\left[\frac{d\mathbf{u}}{d\tau}\right]^2+\int_0^N d\tau\,\lambda(\tau)(\mathbf{u}^2-1)\ . \quad (7.1)$$

Minimization of Eq. (7.1) produces

$$\ddot{u}_i=\lambda u_i\ . \quad (7.2)$$

The Lagrange multiplier λ can be determined now using the fact that

$$\frac{d}{d\tau}\left[\sum_i u_i^2\right]=0\ , \quad (7.3)$$

or

$$\mathbf{u}\cdot\dot{\mathbf{u}}=0\ , \quad (7.4)$$

with the overdot being the usual scalar product. Using Eq. (7.4) we then obtain

$$\frac{d}{d\tau}\mathbf{u}\cdot\dot{\mathbf{u}}=\dot{\mathbf{u}}\cdot\dot{\mathbf{u}}+\mathbf{u}\cdot\ddot{\mathbf{u}} \quad (7.5)$$

while using Eq. (7.2) we have the simple relation

$$\mathbf{u}\cdot\ddot{\mathbf{u}}=\lambda\ . \quad (7.6)$$

The combined use of Eqs. (7.2), (7.5), and (7.6) produces

$$\ddot{u}_i=-(\dot{\mathbf{u}}\cdot\dot{\mathbf{u}})u_i\ . \quad (7.7)$$

We generalize this result by including quadratic perturbations, e.g., such as the "nematic type" in Eqs. (3.8), (3.9) which leads to an equation of motion having the form

$$\ddot{u}_i=\lambda u_i-g_i u_i\ , \quad (7.8)$$

where anisotropic perturbations in all Cartesian directions are included for generality. By using Eqs. (7.5) and (7.8) we obtain

$$\lambda=(\mathbf{g}\mathbf{u})\cdot\mathbf{u}-\dot{\mathbf{u}}\cdot\dot{\mathbf{u}}\ , \quad (7.9)$$

where g is the diagonal matrix

$$\mathbf{g}=\begin{bmatrix} g_1 & 0 & 0\\ 0 & g_2 & 0\\ 0 & 0 & g_3\end{bmatrix}\ .$$

Substitution of Eq. (7.9) into Eq. (7.8) produces

$$\ddot{u}_i=(\mathbf{g}\mathbf{u})\cdot\mathbf{u}u_i-\dot{\mathbf{u}}\cdot\dot{\mathbf{u}}u_i-g_iu_i\ . \quad (7.10)$$

If the term $\dot{\mathbf{u}}\cdot\dot{\mathbf{u}}$ were zero (or constant), then the equation obtained would become a nonlinear Schrödinger equation, which is well studied in the theory of solitons [23]. Remarkably, the problem described by Eq. (7.10) was solved exactly already in 1859 [32] and is known in the mathematical literature as the Neumann problem (or Neumann model). Following [66], let us rewrite Eq. (7.8) in the equivalent form

$$\frac{d^2}{dx^2}\mathbf{s}+\mathbf{g}\mathbf{s}=\lambda\mathbf{s},\quad \mathbf{s}^2=1 \quad (7.11)$$

where obvious redefinitions have been made. Next, we rewrite Eq. (7.11) as

$$\left[\mathbf{s}\wedge\left[\frac{d^2}{dx^2}\mathbf{s}+\mathbf{g}\mathbf{s}\right]\right]=\mathbf{0} \quad (7.12)$$

since $[\mathbf{s}\wedge\lambda\mathbf{s}]=\mathbf{0}$. Let us recall that the Landau-Lifshitz (LL) equation in the theory of ferromagnetism can be written as [67]

$$\frac{\partial}{\partial t}\mathbf{s}=\left[\mathbf{s}\wedge\left[\frac{d^2}{dx^2}\mathbf{s}+\mathbf{g}\mathbf{s}\right]\right],\quad \mathbf{s}^2=1\ . \quad (7.13)$$

Equation (7.12) represents the *static* case of the LL equation *and the traditional hairpin calculations are special cases of the LL equation.* Let us now consider a time-dependent case of the LL equation.

Following [66], let us look for a special type of solution in the form $\mathbf{s}(x,t)=\mathbf{u}(c-i\theta t)$. Using this form in Eq. (7.13) we obtain

$$-i\theta\dot{\mathbf{u}}=[\mathbf{u}\wedge(\ddot{\mathbf{u}}+\mathbf{g}\mathbf{u})],\quad \mathbf{u}^2=1\ . \quad (7.14)$$

Taking the vector product of both sides of Eq. (7.14) we obtain

$$\ddot{\mathbf{u}}+\mathbf{g}\mathbf{u}=\lambda\mathbf{u}+i\theta[\dot{\mathbf{u}}\wedge\mathbf{u}]\ , \quad (7.15)$$

where λ, as before, is given by Eq. (7.9). Equation (7.15) is *the same* as the equation which can be obtained at the classical level from Eq. (6.1) (with $\mathbf{p}=\mathbf{0}$ and quadratic interaction term included) and describes the motion of a charged particle in the presence of the Dirac magnetic monopole [63]. This problem (at the classical level) was solved *exactly* in 1892 by Kötter [33]. At the quantum level, it would correspond to a special case of solutions to the quantum version of the LL equation. Both the classical and the quantum versions of the Neumann model were recently reconsidered [68] and the existing mathematical literature on the classical Neumann model alone is enormous (e.g., see [69], and references therein). At the same time, the quantum Neumann model was only recently formulated [68,70] but not solved. In view of their perturbative nature, the derivations presented in Secs. V and VI are not identical to that given in Refs. [68,70]. It would be of interest to establish the correspondence. This is left for further work. In addition, Kötter's problem falls into the category of Neumann's. This is so, because of the following observation. In the absence of quadratic perturbations, the classical Hamiltonian of our problem is that for the fully symmetric top, e.g., see Eq. (6.16). In the presence of quadratic interactions the total Hamiltonian for Neumann's model can be written as

$$H^t=\tfrac{1}{2}[\mathbf{M}^2+\mathbf{u}\cdot\mathbf{g}\mathbf{u}] , \tag{7.16}$$

provided that the Poisson brackets are

$$\begin{aligned}\{M_i,M_j\}&=\varepsilon_{ijk}M_k ,\\ \{M_i,u_j\}&=\varepsilon_{ijk}u_k ,\\ \{u_i,u_j\}&=0 ,\end{aligned} \tag{7.17}$$

where $\mathbf{M}$ is the angular momentum.

For the Dirac monopole problem, following [66] one can introduce the total angular momentum via

$$\mathbf{M}=[\ddot{\mathbf{u}}\wedge\mathbf{u}]+i\theta\mathbf{u} . \tag{7.18}$$

In terms of the total momentum the commutation relations, Eq. (7.17), remain the same. Complete solution of the classical Dirac monopole problem is given in [66]. It involves the ratios of the elliptic θ functions and will be analyzed elsewhere. Here, we briefly comment on some physical aspects of this problem. It can be easily shown that the system of Eqs. (7.8) supplemented with the constant $\sum_i u_i^2=1$ can be obtained from the Hamiltonian:

$$H=\tfrac{1}{2}\sum_{i=1}^{3} g_i u_i^2+\tfrac{1}{2}[\mathbf{u}^2\mathbf{y}^2-(\mathbf{u}\cdot\mathbf{y})^2] . \tag{7.19}$$

The Hamiltonian equations can now be written as

$$\begin{aligned}\dot{u}_i&=y_i ,\\ \dot{y}_i&=-g_iu_i-u_i\left[\sum_k (g_ku_k^2-y_k^2)\right] ,\end{aligned} \tag{7.20}$$

which obviously coincide with Eq. (7.10). It is easy to show that the auxiliary variable y_k is chosen in such a way that the combination $\sum_k u_k y_k$ is time independent if $\sum_i u_i^2=1$ [69]. So that if initially $\sum_k u_k y_k=0$, then for all times u and y are orthogonal. It can be shown as well [65,69], that the Neumann model has three independent integrals of motion given by

$$F_k=u_k^2+\sum_{i\neq k}\frac{(u_ky_i-u_iy_k)^2}{g_i-g_k},\quad k=1-3 . \tag{7.21}$$

It is less obvious that H obeys the relation

$$H=\tfrac{1}{2}\sum_i a_iF_i . \tag{7.22}$$

The most spectacular result based on Eq. (7.22) lies in the fact that, upon canonical transformation [65]

$$u'=y,\quad y'=-u \tag{7.23}$$

the new Hamiltonian is given by

$$H'=\sum_{i=1} a_i^{-1}F_i \tag{7.24}$$

provided that in these new coordinates the spherical constraint is transformed into that for the ellipsoid:

$$\sum_i \frac{u_i^2}{a_i}=1 . \tag{7.25}$$

From this, effectively, the Neumann model is reduced now to that of Jacobi (for rotation of the ellipsoid) which has a classical solution in terms of the elliptic functions that is well documented in classical mechanics texts. This connection explains why Neumann was able to solve this problem at the classical level more than one hundred years ago.

VIII. DISCUSSION: HOW THE HAIRPIN PROBLEM SOLVES RELATED PROBLEMS IN CONDENSED MATTER AND PARTICLE PHYSICS

In this section we mention briefly hairpinlike problems in various areas of physics (not discussed in the main text) which mathematically are all interrelated. Begin with the classical n-component one-dimensional Heisenberg model [40]. This model is believed to be exactly solvable only in the limit of zero external magnetic field and only for the case when $J_x=J_y=J_z=J$, e.g., see Eq. (3.6). The results presented in the preceding sections provide alternative ways of treating the classical 1D Heisenberg models. It is known [66] that the Neumann and Kötter models originally came from two seemingly unrelated areas: celestial mechanics and mechanics of rotating asymmetric rigid bodies in nonviscous fluids. Quantum versions of these problems lead to the consideration of the rotational Brownian motion of axiasymmetric bodies in fluids. (A review of theoretical results on the rotation of rigid bodies in fluids can be found in [71].) We believe that the results obtained in this paper could be helpful in developing rheological models of suspensions of aspherical particles. If the constraint on the rigidity of a rotating body is removed, then we may have something like the time-dependent LL equation at the classical level. At the quantum level the addition of an extra "time" variable converts our one-dimensional problem to that normally discussed in the context of Wess-Zumino-Novikov-Witten (WZNW) models [72]. In fact, as it is shown in [72], at the classical level the spherical top is just a zero mode of the WZNW model and the classical mechanics treatment of a top parallels that of the WZNW model. The Neumann (Kötter) problem becomes the problem of classical (quantum) deformation of the corresponding Lie groups, as emphasized in [72]. In view of Eq. (5.7), yet another relation can be found. Indeed, if we wrote the corresponding path integral for Eq. (5.7), and generalized the result to include the time dependence, we would obtain a sine-Gordon field theory. In Sec. III we emphasized the connection between the XXZ and the massive Thirring model. This implies that sine-Gordon and Thirring models are equivalent, a result established previously by Coleman [73] using different methods. Because of this equivalence, the bosonization of the Thirring model is possible, and this is related to the fact that the Dirac propagator, given by Eq. (6.1), is expressible in purely bosonic language (i.e., without the use of the conventional Grassmann variables). This fact has its implications in string theory [74] where the newly proposed version of the rigid string includes a sort of nematiclike coupling similar to that used in this work. The rigid string model thus becomes a straightforward two-dimensional generalization of the de Gennes hairpin model. The de Gennes hairpin model has been used in particle physics for some time. For example, in [75] the O(3) nonlinear σ model in $1+1$ dimensions was modified (in the style of de Gennes) to study baryon- and lepton-number violation in the standard electroweak theory. Equation (A15) of [75] is exactly the same as in the Warner-Gunn-Baumgärtner [15] model for hairpins with similar implications and interpretation.

ACKNOWLEDGMENTS

We have benefited from friendly and stimulating discussions with Dr. Udo Seifert (Jülich). The financial support (of A.L.K.) of this work through a DAAD grant is gratefully acknowledged.

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