Nonlinear elastic theory of smectic liquid crystals

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We consider the long-wavelength behavior of smectic liquid crystals (or any solid developing periodic order in only one direction) in the presence of anharmonic terms dictated by symmetry considerations. We analyze this anharmonic model of smectics with the use of analytic renormalization-group techniques directly in three dimensions. We find that the hydrodynamic description of smectics given by the harmonic theory is not valid at sufficiently small wave vectors. Instead, the elastic constants corresponding to the compression and undulation modes, respectively, vanish and diverge logarithmically at small wave vectors. Density correlations, which decay algebraically in the harmonic theory, are found to fall off with a distance-dependent power law at sufficiently long distances. Additionally, the system responds nonlinearly to applied stress at sufficiently small stress, i.e., Hooke's law is not valid. After presenting the calculations leading to the above results, we discuss the feasibility of experimental observation of these effects.

I. INTRODUCTION

Some forty years ago, Landau¹ and Peierls² demonstrated theoretically that three-dimensional crystals whose density is a function of only one spatial coordinate cannot exist. Thermal fluctuations destroy any long-range density order in such "onedimensional" (1D) solids, restoring the uniform density of the liquid state. This result is based on a harmonic description of the 1D solid (i.e., a theory quadratic in displacements about the perfect solid) which involves two elastic constants B and K_1 (here we adopt the notation conventionally used to describe smectic-A liquid crystals³) corresponding to compressional and undulational modes, respectively (see Fig. 1). Subsequently, using this harmonic theory, Caillé⁴ showed that while the density in a 1D solid is uniform, density correlations decay algebraically and not exponentially as would occur in a true liquidlike state. Thus, 1D solids can exhibit quasilong-range order, similar to the ordering found in two-dimensional superfluids and magnets. Indeed, Caille found that the density-density correlation function $G(\vec{x})$ decays as

$$
G(z, x_1 = 0) \sim |z|^{-\eta(t)}, \tag{1.1}
$$

$$
G(z=0,x_1)\sim x_1^{-2\eta(t)},
$$

26

for large $|\vec{x}|$ where η is a continuous function of temperature. (Here z is taken as the direction of the 1D density wave, and the system is cylindrically symmetric about this axis.) In the language of the renormalization group (RG), the continuously varying exponent η arises from the existence of a fixed line in the harmonic (Gaussian spin-wave) approximation. 6.7 Experimental results⁸ for smectic liquid crystals, physical realizations of 1D solids, are consistent with Caillé's prediction (1.1).

In a recent paper, 9 we noted that symmetry arguments require the existence of terms higher than quadratic order (i.e., anharmonic) in the elastic energy of a 2D solid. These anharmonic terms do not

FIG. 1. Two long-wavelength modes of a 1D solid. The dotted lines denote the unperturbed positions of the layers. (a) Compressional: The wave vector of the fluctuation is parallel to the z axis. (b) Undulational: The wave vector of the fluctuation lies in the xy plane.

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modify the qualitative nature of the Landau-Peierls result, however, using analytic RG techniques we showed that these terms are marginally irrelevant with respect to the fixed line of the harmonic theory. In consequence, we showed that the elastic "constants" B and K_1 , respectively, vanish and diverge logarithmically at small wave vector k. We also found that $G(z,x_1=0) \sim |z|^{-y}$ with $y = \eta(T)(\ln z)^{\tilde{\eta}}$ at large z (a similar result holding in the x_1 direction) and $\tilde{\eta}$ takes the universal value $\frac{1}{5}$ [compare with the harmonic result (1.1)]. These results are manifest at sufficiently long wavelengths and our analysis yielded the crossover length scale where the harmonic behavior is replaced by the full anharmonic results.

In this paper, we present the details of the analysis leading to our results. We also present two new calculations: the dependence of $B(k)$ and $K_1(k)$ on *arbitrary* values of $|k_z|/k_1^2$, where $k_1^2 = k_x^2 + k_y^2$, allowing comparison of our predic tions with experiments¹⁰ performed when both k_1 and k_z are nonzero; and the behavior of B as a function of applied stress, which is relevant to mechanical measurements 11 on smectic liquid crystals.

This paper is organized as follows: Section II defines the anharmonic elastic energy describing the 1D solid and explains its origins in terms of symmetry arguments and classical elasticity theory; Sec. III contains the RG analysis of the model; Sec. IV is devoted to a summary of our results and a discussion of the feasibility of their experimental verification. The appendixes contain technical details of the RG analysis.

II. MODEL

The elastic free-energy functional describing a 1D solid can be deduced using symmetry arguments. We require that this energy functional depend only on gradients of $m(\vec{x})$, the spatially varying part of the mass density $n(\vec{x})$, i.e., $n(\vec{x})=n(0)+m(\vec{x})$, where $n(0)$ is the average density. Requiring that the density order at wave vectors \vec{q} for which $|\vec{q}| = q_0$, and that we respect spatial isotropy, we obtain the following free energy:

$$
H = \frac{1}{2} K \int d^3x \{ -2q_0^2 [\vec{\nabla} m(\vec{x})]^2 + [\nabla^2 m(\vec{x})]^2 + O((\nabla^3 m)^2) \} \qquad (2.1)
$$

for some parameter K . Assuming that the 1D solid orders along the z axis with unperturbed layers lying parallel to the $x - y$ plane we write

$$
m(\vec{x}) = \text{Re}\{A(\vec{x})\text{expiq}\left[z + u(\vec{x})\right]\}.
$$

The function $u(\vec{x})$ describes the vertical displacement of a point \vec{x} about its unperturbed position. Transverse displacements corresponding to stretching the layers can be shown to be irrelevant to the long-wavelength behavior of a 1D solid. Using the above expression for $m(\vec{x})$ in (2.1) and neglecting fluctuations in $A(\vec{x})$ [i.e., taking $A(\vec{x})=A$, a constant¹²] we arrive at the spin-wave¹³ Hamiltonian,

$$
H_{\rm sw} = \frac{1}{2t} \int d^3x \left[C \left(\frac{\partial u}{\partial z} \right) + \frac{1}{2} C (\vec{\nabla} u)^2 + \lambda^2 (\nabla^2 u)^2 + \left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial z} \right) (\vec{\nabla} u)^2 + \frac{1}{4} [(\vec{\nabla} u)^2]^2 \right],
$$
 (2.2)

where $t \equiv [4K(Aq^2)^2]^{-1}$, $C \equiv q^{-2}(q^2 - q_0^2)$, and λ is proportional¹⁴ to q^{-1} . The value of C and hence q (the wave vector of the 1D density wave) is determined by demanding that the expectation value $\langle \partial u / \partial z \rangle = 0$, thus ensuring that we perturb about a configuration of stable equilibrium. This choice for C also guarantees that $\langle (\vec{\nabla}_\mu)^2 \rangle = 0$ where, $\nabla_1^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. (See Appendix A for an explicit one-loop verification of this result.)

Equation (2.2) can also be obtained on the basis of classical elasticity theory.¹⁵ Since the displace ments of the particles of the 1D solid are assumed to be one dimensional, the trace of the Lagrangian strain tensor 16 reduces to

$$
\text{Tr}\overrightarrow{e} = \frac{\partial u}{\partial z} + \frac{1}{2}(\vec{\nabla}u)^2.
$$
 (2.3)

Since the 1D solid cannot support shear, the elastic free energy is a function only of the invariant $Tr\vec{e}$ and the bending (i.e., undulational energy density $(\nabla^2_{\mu}u)^2$. Thus, we can write the free energy as

$$
H = \frac{1}{2t} \int d^3x [C(Tt\vec{e}) + (Tt\vec{e})^2 + \lambda^2 (\nabla_1^2 u)^2
$$

+ O((Tt\vec{e})^3)], (2.4)

which is identical to (2.2), aside from a term $\lambda^2(\partial u^2/\partial z^2)^2$ which can be neglected at long wavelengths. As noted above, we choose C so that $\langle \partial u / \partial z \rangle = 0$. This condition is simply the statement that the thermal average of the strain is zero in the absence of applied stress.

If we drop higher than quadratic terms in u in (2.2) we arrive at the Gaussian or harmonic approximation. To obtain $\langle \partial u / \partial z \rangle = 0$ we must choose $C=0$, and Fourier transforming we find for small k

$$
H_{\rm sw} \sim \frac{1}{2t} \int d^3k [k_z^2 + \lambda^2 (k_\perp^4)] |u(\vec{k})|^2.
$$
 (2.5)

The coefficients of k_z^2 and k_{\perp}^4 in (2.5) are, respectively, B/k_BT and K_1/k_BT . Using (2.5) one can readily establish the Landau-Peierls instability, i.e., $\langle m(\vec{x}) \rangle = 0$, as follows:

$$
\langle m(\vec{x}) \rangle = A \langle \expiq[z + u(\vec{x})] \rangle
$$

= $A \exp(iqz) \exp[-\frac{1}{2} \langle u^2(\vec{x}) \rangle]$. (2.6)

By the equipartition theorem

$$
\langle u^2(\vec{x})\rangle = \int d^3k \frac{t}{k_z^2 + \lambda^2 k_\perp^4} \to \infty
$$
 (2.7)

when $t\neq0$ for a system of infinite size; hence, $\langle m(\vec{x}) \rangle = 0$, unless $t = 0$. One can also recover the results of Caillé⁴ for $G(\vec{x})$ [see (1.1)] with $\eta(t) = q^2 t / 8 \pi \lambda$.

The necessity of anharmonic terms in (2.2) can be understood in terms of the rotational isotropy of the system. If one begins with an unperturbed 1D solid (i.e., $u = 0$) and uniformly rotates the system by an angle θ about, for example the y axis, one generates a displacement

$$
u(\vec{x}) = z(\cos\theta - 1) + x\sin\theta.
$$
 (2.8)

It is straightforward to verify that upon substituting (2.8) in (2.2) one obtains $H_{sw}=0$ identically. However, with only quadratic terms present, $H_{sw} = O(\theta^4)$. Thus, anharmonic terms are required to preserve the rotational invariance for arbitrarily large uniform rotations.

III. RG ANALYSIS AND CROSSOVER BEHAVIOR

A. Renormalization program

To assess the effects of the anharmonic terms in (2.2) we employ the field-theoretic RG techniques of Brézin et al.¹⁷ Our analysis will follow closely an earlier study⁷ of the spin-wave Lifshitz point model which contains a single anharmonic term proportional to $[(\vec{\nabla}_1 u)^2]^2$. The quadratic theory (2.5) is used as the noninteracting Hamiltonian, and the anharmonic terms are treated perturbatively in powers of t. The calculation is simplified by rescaling the field $u(\vec{x})$ and the coordinates \vec{x} as follows:

$$
u(\vec{x}) = \left(\frac{t}{\lambda}\right)^{1/2} \psi(\tilde{\vec{x}}),
$$

$$
\vec{x}_1 = \tilde{\vec{x}}_1,
$$

$$
z = \lambda^{-1}\tilde{z},
$$
 (3.1)

where the field ψ is dimensionless. With this rescaling (note that $d^3x = \lambda^{-1} d^3\tilde{x}$), Hamiltonian (2.2) takes the form

$$
H = \int \frac{d^3 \tilde{x}}{2} \left[\frac{C}{\lambda^{1/2} t^{1/2}} \frac{\partial \psi}{\partial \tilde{z}} + \frac{C}{\lambda^2} (\tilde{\vec{\nabla}}_1 \psi)^2 + \left[\frac{\partial \psi}{\partial \tilde{z}} \right]^2 + (\tilde{\nabla}_1^2 \psi)^2 + \left[\frac{t}{\lambda^3} \right]^{1/2} \left[\frac{\partial \psi}{\partial \tilde{z}} \right] (\tilde{\vec{\nabla}}_1 \psi)^2 + \frac{1}{4} \left[\frac{t}{\lambda^3} \right] [(\tilde{\vec{\nabla}}_1 \psi)^2]^2 \right],
$$
\n(3.2)

where we have dropped terms proportional to $(\partial_z^2 \psi / \partial \tilde{z}^2)^2$, $(\partial \psi / \partial \tilde{z})^3$, $(\partial \psi / \partial \tilde{z})^4$, and $(\vec{\nabla}_1 \psi)^2 (\partial \psi / \partial \tilde{z})^2$ which, by power counting, are irrelevant with respect to the fixed line of the quadratic theory. Since we will ultimately develop a loop expansion in powers of t , we have also dropped a term proportional to $C(\partial \psi / \partial \tilde{z})^2$ (recall that $C = 0$ in the quadratic theory). The two anharmonic terms displayed in (3.2) are marginal by powercounting arguments, and we define a dimensionless coupling

$$
w_0 \equiv \frac{t}{\lambda^3} \tag{3.3}
$$

To suppress the infrared divergences in perturbation theory in powers of w_0 , we add a mass term $\frac{1}{2}m_0^2\psi^2$ to (3.2), letting $m_0 \rightarrow 0$ at the end of the RG calculation. Multiplicative renormalizability of the twopoint correlation function $g(\vec{k}_1, k_z) = \langle \psi(\vec{k}) \rangle$ $\times\psi(-\vec{k})$ requires that there exist dimensionless renormalization constants Z_{ψ} , Z_{m} , and Z_{w} such that in the limit where the ultraviolet cutoff $\Lambda \rightarrow \infty$, the quantity

remains finite order by order in w_0 when expressed in terms of the renormalized variables w and k_z^R defined by 18

$$
w_0 = Z_w w \t{3.4a}
$$

$$
k_z = Z_m k_z^R \tag{3.4b}
$$

Similar statements of renormalizability can be made for the vertices $\Gamma_3(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ and $\Gamma_4(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4)$, the amputated Fourier transforms of the connected, single-particle irreducible three-point and four-point correlation functions, respectively. Specifically,¹⁹ we require that the quantities $Z_m^{3/2} Z_\psi^{3/2} Z_\psi^{1/2} \Gamma_3$ and $Z_w Z_\psi^4 Z_m \Gamma_4$ remain finite as $\Lambda \rightarrow \infty$ when expressed in terms of the renormalized variables. As described in Sec. II, the parameter C in (3.2) is chosen to ensure that $\langle \partial \psi / \partial \tilde{z} \rangle = 0$; C is therefore treated as a renormalization constant, not as an independent coupling constant.

B. RG equations: $g^{-1}(\vec{k})$ in the absence of applied stress

The explicit computations with Hamiltonian (3.2) of $g^{-1}(\overline{k})$, Γ_3 , and Γ_4 are summarized in Appendi A where expressions for Z_w , Z_m , and Z_w , which render the theory finite, are given to first order in w_0 . By dimensional analysis, the correlation function $g^{-1}(\vec{k}_1, k_2, w_0, \Lambda)$ can be written in the form

$$
g^{-1}(\vec{k}_1, k_2, w_0, \Lambda) = k_z^2 f\left(\frac{\Lambda}{R_0}, S_0, w_0\right), \qquad (3.5)
$$

where the dimensionless quantities $\Lambda^{-1}R_0$ and S_0 are given by

$$
\Lambda^{-1}R_0 = \Lambda^{-1} \left[k_z^2 + k_\perp^4 \right]^{1/4}, \tag{3.6a}
$$

$$
S_0 = \frac{k_z}{k_\perp^2} \tag{3.6b}
$$

Renormalizability of the theory implies that the function f satisfies the RG equation:

$$
\frac{\partial}{\partial l} - \frac{1}{2} \frac{\gamma_1}{1 + S_0^{-2}} \frac{\partial}{\partial l} + \gamma_1 S_0 \frac{\partial}{\partial S_0} + \beta_w \frac{\partial}{\partial w_0}
$$

$$
+ 2\gamma_\psi + 2\gamma_1 \left| f \left(\frac{\Lambda}{R_0}, S_0, w_0 \right) \right| = 0 , \quad (3.7)
$$

where $l = \ln(\Lambda/R_0)$, m_0 has been set equal to zero, and

$$
\gamma_1 \equiv \frac{1}{k_z} \frac{\partial k_z}{\partial l} \bigg|_{k_z^R} = \frac{\partial \ln Z_m}{\partial l} \bigg|_{w} = \frac{3w_0}{64\pi} + O(w_0^2) , \qquad (3.8a)
$$

$$
\beta_w \equiv \frac{\partial w_0}{\partial l} \bigg|_w = \frac{5w_0^2}{64\pi} + O(w_0^3) , \qquad (3.8b)
$$

$$
\gamma_{\psi} = \left. \frac{\partial \ln Z_{\psi}}{\partial l} \right|_{w} = \frac{-w_0}{64\pi} + O(w_0^2) \ . \tag{3.8c}
$$

To lowest order in w_0 , the solution of (3.7) is given bv^{17}

$$
f\left[\frac{\Lambda}{R_0}, S_0, w_0\right] = f(1, \widetilde{S}(l), \widetilde{w}(l)) \exp\left[-2\int_0^l \{\gamma_{\psi}[\widetilde{w}(\tau)] + \gamma_1[\widetilde{w}(\tau)]\} d\tau\right],
$$
\n(3.9)

where \tilde{S} and \tilde{w} are functions of S_0 , w_0 , and τ determined by the RG flow equations

$$
\frac{\partial \widetilde{S}}{\partial \tau} = -\widetilde{S}\gamma_1(\widetilde{w})\;, \tag{3.10a}
$$

$$
\frac{\partial \widetilde{w}}{\partial \tau} = -\beta_w(\widetilde{w}) \tag{3.10b}
$$

and the boundary conditions $\tilde{S}(\tau=0)=S_0$, and $\tilde{w}(\tau=0)=w_0$. Using (3.8a) and (3.8b) the solutions of (3.10) with the above boundary conditions are found to be

$$
\widetilde{S} = S_0 \left[1 + \frac{5w_0}{64\pi} \tau \right]^{-3/5},
$$
\n(3.11a)

$$
\widetilde{w} = w_0 \left[1 + \frac{5w_0}{64\pi} \tau \right]^{-1} . \tag{3.11b}
$$

The function $f(1,\tilde{S}(l),\tilde{w}(l))$ is evaluated in a regime where the Gaussian theory is valid [i.e., $\tilde{w}(l) \ll 1$], and thus to zeroth order in $\tilde{w}(l)$ we have

$$
f(2,\widetilde{S}(l),\widetilde{w}(l)) = 1 + [\widetilde{S}(l)]^{-2} . \tag{3.12}
$$

Using {3.5), (3.9), (3.11), and (3.12) we then find

$$
g^{-1}(\vec{k}_1, k_z, w) \sim k_z^2 \left[1 + \frac{5w}{64\pi} \ln \frac{\Lambda}{(k_z^2 + k_\perp^4)^{1/4}} \right]^{-4/5} + k_\perp^4 \left[1 + \frac{5w}{64\pi} \ln \frac{\Lambda}{(k_z^2 + k_\perp^4)^{1/4}} \right]^{2/5} .
$$
 (3.13)

Equation (3.13) implies the existence of crossover length scales $(k_1^*)^{-1}$ and $(k_2^*)^{-1}$ satisfyin

$$
(k_z^*)^2 + (k_\perp^*)^2 = \Lambda^{-4} \exp\left[\frac{256\pi}{5w}\right],\tag{3.14}
$$

where the system crosses over from the familiar Gaussian behavior to the asymptotic behavior governed by the full Hamiltonian (3.2). In the Gaussian regime, $k_z^2 + k_{\perp}^4 \gg (k_z^*)^2 + (k_{\perp}^*^2)^2$ and $g^{-1}(\vec{k}_1, k_z) \sim k_z^2 + (k_{\perp}^2)^2$. For $k_z^2 + k_\perp^4 \ll (k_z^*)^2 + (k_\perp^*^2)^2$, however, (3.13) yields

$$
g^{-1}(\vec{k}_1, k_z) \sim k_z^2 \left[\ln \frac{\Lambda}{(k_z^2 + k_1^4)^{1/4}} \right]^{-4/5} + k_\perp^4 \left[\ln \frac{\Lambda}{(k_z^2 + k_1^4)^{1/4}} \right]^{2/5}.
$$
 (3.15)

We can define renormalized elastic constants $B^R(\vec{k})$ and $K_1^R(\vec{k})$ as the coefficients of $k_z^2/k_B T$ and $k_\perp^4/k_B T$ in $g^{-1}(\vec{k})$, respectively. Hence, one sees from (3.15) that $B^R(\vec{k})$ and $K_1^R(\vec{k})$, respectively, vanish and diverge logarithmically at small k , implying the breakdown of hydrodynamics in the asymptotic regime.

C. RG equation: $g^{-1}(\vec{k})$, in the presence of applied stress

In the presence of an externally-applied dilative stress σ_0 , we add a term¹⁵

$$
\frac{\sigma_0}{k_B T} \int d^3x \frac{\partial u}{\partial z}
$$

to the Hamiltonian (2.2). With the rescaling (3.1) this term becomes

$$
\frac{\sigma_0}{k_BT}\left(\frac{t}{\lambda}\right)^{1/2}\int d^3x\frac{\partial\psi}{\partial\widetilde{z}}.
$$

If we let $C \rightarrow C + (\sigma_0 t / k_B T)$ then the symmetrybreaking term in the Hamiltonian becomes

$$
-\frac{1}{2}v_0^2\int d^3\tilde{\mathbf{x}}(\tilde{\vec{\nabla}}_1\psi)^2\,,\tag{3.16}
$$

where $v_0^2 = \sigma_0 t / \lambda^2 k_B T$. Renormalizability of the theory in the presence of (3.16) implies that $Z_{\psi}^2 g^{-1}(k)$ is finite as $\Lambda \rightarrow \infty$ when expressed in terms of the renormalized parameters given by (3.4) and by

$$
v_0^2 = Z_v^2 v^2 \tag{3.17}
$$

A calculation of Z_v to first order in w_0 is presented in Appendix A. To this order, $Z_v = Z_m$. Assuming for convenience that $k_{\perp} = 0$, dimensional analysis allows us to write²⁰

$$
g^{-1}(k_z, v, w) = k_z^2 h \left[\ln \frac{\Lambda}{v_0}, w_0 \right],
$$
 (3.18)

where h satisfies the RG equation:

$$
\left(\frac{\partial}{\partial x} - \gamma_1 \frac{\partial}{\partial x} + 2\gamma_1 + 2\gamma_\psi + \beta_w \frac{\partial}{\partial w_0}\right) h(x, w) = 0
$$
\n(3.19)

and $x = \ln(\Lambda/v_0)$. To lowest order, the solution of (3.19) is given by

$$
h(x,w) \sim h(1,\widetilde{w}(x)) \exp \left[-2 \int_0^x {\gamma_1[\widetilde{w}(\tau)] + \gamma_{\psi}[\widetilde{w}(\tau)] } d\tau \right]
$$

with $\tilde{w}(\tau)$ given by (3.11b). We then find that (3.20)

re renormalized parameters given by (3.4)
\n
$$
g^{-1}(k_z, v, w) \sim k_z^2 \left[1 + \frac{5w}{64\pi} \ln \left[\frac{\Lambda}{v_0} \right] \right]^{-4/5}.
$$
\n(3.17)

The above expression for g^{-1} implies the existence of a crossover stress scale defined by

$$
v^* = \Lambda^{-1} \exp\left[\frac{64\pi}{5w}\right].
$$
 (3.22)

Recalling that $B^R / k_B T$ is defined as the coefficient of k_z^2 in g^{-1} , we see that for stresses $v >> v^*$, linearresponse theory (Hooke's Law) is valid, i.e., B^R is independent of stress. However, when $v \ll v^*$,

$$
g^{-1} \sim k_z^2 \left[\ln \left(\frac{\Lambda}{v_0} \right) \right]^{-4/5}
$$

and the system responds nonlinearly to stress.²¹

D. RG equation: $G(\vec{x})$

Techniques similar to those used above in the discussion of $g^{-1}(k)$ can be used to find the large distance behavior of the density-density correlation function $G(\vec{x})$, defined by

$$
G(\vec{x}_1, \tilde{z}, w) = \langle \exp\{i\lambda^{-1} [u(\vec{x}) - u(\vec{0})]\}\rangle
$$

= $\langle \exp\{iu_0[\psi(\tilde{\vec{x}}) - \psi(\tilde{\vec{0}})]\}\rangle$, (3.23)

where $u_0 = w_0^{1/2}$ [under renormalization, however, $u(l)$ differs from $w^{1/2}(l)$. The renormalizability of $G(\vec{x})$ implies that there exists a renormalization constant Z such that ZG is finite in the limit $\Lambda \rightarrow \infty$ when expressed in terms of renormalized quantities. The calculation of Z to first order in w_0 is displayed in Appendix B. By dimensional analysis, G can be written as a function of the dimensionless variables,

$$
\Lambda r_0 = \Lambda (\bar{z}^2 + x_\perp^4)^{1/4} \,, \tag{3.24a}
$$

$$
s_0 = \frac{\widetilde{z}}{x_1^2} \tag{3.24b}
$$

and satisfies the RG equation:

$$
\left[\frac{\partial}{\partial l} - \frac{\gamma_1}{2} \frac{1}{1 + s_0^{-2}} \frac{\partial}{\partial l} - s_0 \gamma_1 \frac{\partial}{\partial s_0} + \beta_w \frac{\partial}{\partial w_0} + \beta_u \frac{\partial}{\partial u_0} + \gamma \right] G = 0 , \quad (3.25)
$$

where $l = \ln(\Lambda r_0)$ and

$$
\beta_u = u_0 \frac{\partial \ln(Z_{\psi}^{-1} Z_m^{-1/2})}{\partial l} \bigg|_{w} = -\frac{w_0 u_0}{128\pi} + O(w_0^2) ,
$$

$$
\gamma = \frac{\partial \ln Z}{\partial l} \bigg|_{w} = \frac{u_0^2}{4\pi} + R' w_0 u_0^4 + O(w_0^2) , \qquad (3.26b)
$$

and R' is a nonuniversal number (i.e., it depends on the specific cutoff procedure used to evaluate the integrals). The solution of (3.24) to lowest order is given by

$$
G(r,s,w) \sim G(1,\tilde{s}(l),\tilde{w}(l))
$$

×
$$
\times \exp\left[-\int_0^l \gamma[\tilde{u}(\tau),\tilde{w}(\tau)]d\tau\right],
$$
\n(3.27)

where $l = \ln(\Lambda r_0)$ and \tilde{u} is a function of u_0 , w_0 , and τ determined by the RG flow equation:

$$
\frac{\partial \widetilde{u}}{\partial \tau} = -\beta_u(\widetilde{u}, \widetilde{w})\tag{3.28}
$$

and the boundary condition $\tilde{u}(\tau = 0) = u_0$. Using $(3.11b)$ and $(3.26a)$ the solution of (3.28) is given by

$$
\widetilde{u} = u_0 \left[1 + \frac{5w_0}{64\pi} \right]^{1/10} . \tag{3.29}
$$

The function $G(1,\tilde{s}(l),\tilde{w}(l))$ is evaluated in the Gaussian regime. Its form for arbitrary values of \tilde{z}/x_1^2 is cumbersome⁴; however, in the limits $\tilde{z} \gg x_1^2$ and $\tilde{z} \ll x_1^2$, $G(1,\tilde{s}(l),\tilde{w}(l))$ behaves like a constant to lowest order. Using (3.26b), (3.27), and (3.29) we conclude that for $\tilde{z} \ll x_1^2$, G scales as

$$
G(\vec{x}) \sim \exp\left\{-\frac{8}{3}\left[\left(1 + \frac{5w}{64\pi}\ln(x_{\perp}\Lambda)\right)^{6/5} - 1\right] - R\left[1 + \frac{5w}{64\pi}\ln(x_{\perp}\Lambda)\right]^{2/5}\right\},\qquad(3.30)
$$

where R is proportional to R'. When $\tilde{z} \gg x_1^2$, $G(\vec{x})$ is given by (3.30) with x_{\perp} replaced by $\tilde{z}^{1/2}$. The crossover length scales are thus given by

$$
x_1^* = (\tilde{z}^*)^{1/2} = \Lambda^{-1} \exp\left(\frac{64\pi}{5w}\right). \tag{3.31}
$$

At distances $x_1 \ll x_1^*$, we recover from (3.30) the

Gaussian result
\n
$$
G(x_1,\tilde{z}=0) \sim x_1^{-w/4\pi}
$$
. (3.32)

However, at distances $x_1 \gg x_1^*$, we find

$$
G(x_\perp, \widetilde{z}=0) \sim x_\perp^n , \qquad (3.33)
$$

(3.26a)

where

$$
n = -\frac{8}{3} \left[\frac{5w}{64\pi} \right]^{6/5} [\ln(x_{\perp} \Lambda)]^{1/5}
$$

$$
-R \left[\frac{5w}{64\pi} \right]^{2/5} [\ln(x_{\perp} \Lambda)]^{-3/5} . \tag{3.34}
$$

When $x_1 = 0, \tilde{z} \neq 0$, $G(\tilde{z})$ is given by $(3.32) - (3.34)$ with x_1 replaced by \tilde{z}^1

IV. DISCUSSION

We have considered the long-wavelength behavior of 1D solids in the presence of the anharmonic terms demanded by rotational symmetry. While some of these terms are irrelevant with respect to the fixed line of the harmonic theory, two terms, namely, $(\nabla_{\perp} u)^2 (\partial_z u)$ and $[(\nabla_{\perp} u)^2]^2$ represent marginal operators. Using analytic RG methods directly in three dimensions we have assessed the effects of these marginal operators, and found the following results:

(1) At sufficiently long wavelengths, the renormalized elastic constants $B^R(\vec{k})$ and $K_1^R(\vec{k})$, respectively, vanish and diverge logarithmically [see (3.15)]. This nonanalytic dependence of the elastic constants on the wave vector k implies that the gradient expansion, whose existence is the central assumption of hydrodynamics, is not valid at sufficiently long wavelengths in 1D solids.

(2) For sufficiently small applied stress, the linear relationship between stress and strain (Hooke's Law) breaks down. This effect is manifest in the nonanalytic dependence of B^R on the applied stress [see (3.21)].

(3) Density correlations decay at sufficiently long distances with a length-dependent power law [see (3.33)].

The crossover length and stress scales [see (3.14), (3.22), and (3.31)] where the above effects begin to dominate the system's behavior are determined by the dimensionless quantity $w = k_B T B^{1/2} / K_1^3$ which serves as the expansion parameter of our perturbative RG procedure. The predicted effects should be observed more readily in liquid crystals with large values of w (i.e., the crossover wave vector and stress scales will be larger in such systems). Since the compressibility B tends to zero or a small constant²³ as the nematic – smectic-A transition is approached from below, the anharmonic behavior should be more easily seen deep in the smectic-A phase. For a typical smectic-A liquid crystal, $T \sim 350 \text{ °K}, K_1 \sim 5 \times 10^{-7} \text{ dyne, }^{24} \text{ and } B \sim 5 \times 10^{-7}$

dyne/cm²,²⁵ whereupon $w \sim 0.7$. Since these numbers are typically obtained through experiments done at wave vectors²⁴ $\Lambda \sim 10^{-3}$ $\rm \AA^{-1}$, we substitute this value for Λ in (3.13). For a light scattering measurement of K_1 , we choose $k_z = 0$ (Ref. 24) and obtain from (3.13)

$$
K_1^R(k_1) = K_1(\Lambda) [1 - 0.017 \ln(10^3 k_1)]^{2/5}, (4.1)
$$

where k_1 is measured in reciprocal angstroms and $K_1(\Lambda) \sim 10^{-6}$ dynes, the value of K_1 at $k_1 \sim \Lambda \sim 10^{-3} \text{\AA}^{-1}$. The elastic constant K_1 can be measured by light scattering with an accuracy of about²⁶ 3%. The logarithmic correction term therefore becomes observable at k_1 's sufficiently small that $K_1^R(k_1)$ and $K_1(\Lambda)$ differ by more than 3%,
i.e., when $k_1 \sim 10^{-5} \text{A}^{-1}$. In light scattering experiments²⁷ k's $\sim 10^{-5}$ Å⁻¹ are obtainable

In the second sound measurement of B reported in Ref. 10, e.g., wave vectors $|k|$ as large as 400 cm^{-1} =40×10⁻⁷ Å⁻¹, and values of k_z as small as 10^{-7} Å⁻¹ can be obtained. Setting²⁸ k_1 = 0 in (3.13) and using $A \sim 40 \times 10^{-7}$ A^{-1} , $k_z = \lambda^{-1} 10^{-7}$ A^{-1} with $\lambda=10$ Å (Ref. 24) and $w = 0.7$, we find

$$
\frac{\delta B}{B(\Lambda)} \equiv \frac{B(k_z) - B(\Lambda)}{B(\Lambda)} = 5\% \tag{4.2}
$$

Reference 10 actually reports hydrodynamic behavior (i.e., constant B) over the available range of k_z 's. However, the data was taken near the nematic – smectic-A transition where B is small; in consequence $w \sim 0.1$ for these measurements and the expected change in B for k_z 's between 10^{-7} and 4×10^{-6} $\rm \AA^{-1}$ is less than 1%.

Estimates for the observability of the nonhydrodynamic behavior are very sensitive to the value of w. For example, given a liquid crystal²⁹ with $w = 4$, a 3% variation in K_1 occurs between $k_1 \sim 10^{-4}$ Å and $k_1 \sim 10^{-3}$ \mathring{A}^{-1} ; the fractional change in B over the range of k_z 's probed in Ref. 10 becomes 36%. In making these estimates one should note that (3.13) was derived assuming $w \ll 1$, and higherorder corrections [i.e., higher powers of w multiplying the logarithmic terms in (3.13)] have been neglected. While such corrections do not alter the form of $g^{-1}(\vec{k})$ [i.e., $k_1^4(\ln k_1)^{2/5}$ or $k_2^2(\ln k_2)^{-4/5}$] for asymptotically small \vec{k} , they can, in principle, affect estimates of the observability of the nonlinear corrections. In ignoring these higher-order terms we have implicitly made the assumption that the true expansion parameter is [see (3.13)] something like $w/64\pi$ rather than simply w, in which case the higher-order terms play no role until w becomes larger than 100.

A similar assessment can be made of the feasibility of observing the breakdown of Hooke's Law, i.e., the nonanalytic dependence of B on the applied stress for small stress. Equation (3.21) for the renormalized elastic constant B^R can, e.g., be cast readily in the form

$$
B^{R}(v) = B^{R}(v_0) \left[1 + \frac{5w(v_0)}{64\pi} \ln \left(\frac{v_0}{v} \right) \right]^{-4/5},
$$
\n(4.3)

where

$$
w(v_0) \equiv \left(\frac{5\ln(\Lambda/v_0)}{64\pi} + w^{-1}\right)^{-1}
$$

is the solution of $(3.10b)$ with the boundary condition $w(\Lambda) = w_0$. Recalling $v = (\sigma t)^{1/2} (\lambda K_B T)^{-1}$ we write (4.3) in terms of the stress σ as

$$
B^{R}(\sigma) = B^{R}(\sigma_0) \left[1 + \frac{5w(v_0)}{128\pi} \ln \left(\frac{\sigma_0}{\sigma} \right) \right]^{-4/5}.
$$
 (4.4)

Again assuming $w(v_0)$ ~ 0.7, one finds, as in (4.2), the percentage change in B^R for a given change in σ :

$$
\frac{\delta B}{B(\sigma_0)} \equiv \frac{B^R(\sigma) - B^R(\sigma_0)}{B(\sigma_0)}
$$

$$
\sim -(0.007)\ln\left(\frac{\sigma_0}{\sigma}\right).
$$
 (4.5)

A fractional change in B of, e.g., 5% is then achieved by changing σ by a factor of about 1000 (i.e., $\sigma_0/\sigma \sim 1000$). In principle, one can indeed measure B over three or four decades of stress. In measure *B* over three or four decades of stress. In
the experiment of Bartolino and Durand,¹¹ for example, stresses and strains in the smectic liquid crystal 8OCB were measured with piezoelectric ceramics. The maximum applied stress was roughly 500 dynes/cm², corresponding to a voltage of about 10^{-3} V across the ceramic. Since one can measure voltages down to the noise level $(10^{-7}$ to 10^{-6} V), three or four decades ought to be accessible. In practice, the factor which limits such experiments on the low-voltage end is probably the finite size of the sample. To understand this observation, note that we have assumed $k_z = 0$ or, more precisely, $v_0 \gg (k_z/\lambda)^{1/2}$, in the argument of the logarithm in (3.21). Recalling that $v_0 \equiv (\sigma_0/B\lambda^2)^{1/2}$ we infer that the stress σ_0 can be lowered unti

$$
\sigma_0 \sim \sigma^* \equiv B\lambda k_z \ , \qquad (4.6)
$$

whereupon further evolution of B is halted by the with

sample's finite size. With $B \sim 5 \times 10^7$ dyne/cm². $\lambda \sim 10^{-7}$ cm, and $k_z \sim 10$ cm⁻¹, we have $\sigma^* \sim 50$ $dyne/cm²$; this represents a decrease by only a factor of 10 from the maximum stress of 500 $dyne/cm²$ in the Bartolino-Durand experiment, and should be accompanied by roughly a 2% decrease in the value of B .

In view of the extreme (exponential) sensitivity of these estimates to the value of the parameter w , it is worth emphasizing that reliable values of both B and K_1 (which determine w) for smectics A far from the $N-A$ transition are simply not available. The "typical" numbers we have used in the above estimates are, in fact, very conservative. For example, $B \sim 5 \times 10^7$ dyne/cm² seems a reasonable number for bilayer smectics,²⁵ but much larger B 's (for example \sim 2 \times 10⁹ dyne/cm²) have been measured in monolayer materials.³⁰ So far as we can ascertain, values of K_1 are not available for these monolayers. If, however, K_1 does not change appreciably from bilayers to monolayers, 31 the monolayers can have values of w almost ten times as large as the $w \sim 0.7$ we have been assuming. In such a material anharmonic effects would be readily observable. Measurements of K_1 in monolayer materials whose B 's are known is, from this point of view, a worthwhile endeavor.

(4.5) ACKNO%LEDGMENTS

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APPENDIX A: COMPUTATION OF THE Z's

The computations of $g^{-1}(\vec{k})$, the inverse Fourier transform of $\langle \psi(\vec{x})\psi(\vec{0})\rangle$, Γ_3 , the three-point vertex, and Γ_4 , the four-point vertex to first order in w_0 are presented here.

I. $g^{-1}(\vec{k})$

Writing Dyson's equation,

$$
g^{-1}(\vec{k}) = g_0^{-1}(\vec{k}) - \Sigma(\vec{k})
$$

$$
g_0^{-1}(\vec{k}) \equiv k_z^2 + (k_\perp^2)^2 + m_0^2,
$$

one generates from (3.2) the diagrammatic perturbation series for $\Sigma(k)$ shown in Fig. 2. Only diagrams divergent as the inverse ultraviolet cutoff a tends to zero have been included; the Z's are chosen to remove these divergences in each order of the expansion in w_0 . The graph in Fig. 2(a) yields the following divergent quantity:

$$
\Sigma_a(k) = k_z^2 \frac{w_0 \ln \Lambda}{16\pi} + k_\perp^2 \frac{w_0 \ln \Lambda}{8\pi} + k_\perp^4 \frac{w_0 \ln \Lambda}{32\pi}
$$
\n(A1)

while the graph in Fig. 2(b) yields

$$
\Sigma_b(k) = -k_1^2 \frac{w_0 \ln \Lambda}{4\pi} \ . \tag{A2}
$$

We choose C in (3.2) to cancel the $O(k_1^2)$ terms in $(A1)$ and $(A2)$. This same choice of C cancels the graph of Fig. 3, thus ensuring that $\langle \partial \psi / \partial \tilde{z} \rangle = 0$ to this order. In the presence of an external stress (3.16), an additional contribution to $\Sigma(k)$ comes from the graphs of Fig. 4, which yield the divergent quantity

$$
\Sigma_v = -k_1^2 w_0 v_0^2 \frac{\ln \Lambda}{16\pi} \ . \tag{A3}
$$

Note that $g_0^{-1}(k)$ now includes a term $-v_0^2k_1^2$.

Thus, we find to first order in w_0 ,

$$
g^{-1}(k) = k_z^2 \left[1 - \frac{w_0 \ln \Lambda}{16\pi} \right] + k_\perp^4 \left[1 + \frac{w_0 \ln \Lambda}{32\pi} \right]
$$

$$
-v_0^2 k_\perp^2 \left[1 - \frac{w_0 \ln \Lambda}{16\pi} \right].
$$
 (A4)

The renormalizability assumption demands that the substitutes (3.4) and (3.17) render the quantity $Z_{\psi}^2 g^{-1}(k)$ finite. This assumption yields

$$
Z_{\psi} = 1 - \frac{w_0 \ln \Lambda}{64\pi} , \qquad (A5a)
$$

$$
Z_v = Z_m = 1 + \frac{3w_0 \ln \Lambda}{64\pi} \ . \tag{A5b}
$$

FIG. 2. Graphs contributing to the self-energies Σ_a and Σ_b . Each solid line represents a bare propagator $g_0(k)$.

FIG 3. Graph contributing to $\langle \partial \psi / \partial z \rangle$.

II. Γ_3 and Γ_4

The vertices $\Gamma_3(k_1, k_2, k_3)$ and $\gamma_4(k_1, k_2, k_3, k_4)$ are the amputated Fourier transforms of the connected, single-particle irreducible three-point and four-point correlation functions, respectively. To compute Z_{ω_2} one need only compute the part of $\Gamma_3(k, k, -2k)$ proportional to $k_z(k_1)^2$, and the part of $\Gamma_4(\vec{k}, \vec{k}, -\vec{k}, -\vec{k})$ proportional to $(\vec{k}_1^2)^2$. Diagrams contributing to these quantities appear in Fig. 5. Evaluation of these diagrams leads to the results

$$
\Gamma_3 \sim \frac{\sqrt{w_0}}{2} \left[1 - \frac{w_0 \ln \Lambda}{16\pi} \right], \qquad (A6a)
$$

$$
\Gamma_4 \sim \frac{w_0}{8} \left[1 - \frac{w_0}{16\pi} \ln \Lambda \right].
$$
 (A6b)

The appropriate combinations of Z's rendering Γ_3 and Γ_4 finite are found by relating these vertices and $g(\vec{k})$ to the corresponding functions in the unscaled theory (2.2) . Using (3.1) we find that

$$
w^2\lambda^3\Gamma_4(\vec{k}_{\perp},k_z) = \Gamma_4'(\vec{k}_{\perp},\lambda k_z)
$$

where Γ'_4 is the vertex function associated with the Hamiltonian (2.2). Likewise, the Fourier transforms of the two-point correlation functions expressed in terms of ψ and u, respectively, are related by $g(\vec{k}_1, k_z) = g'(\vec{k}_1, \lambda k_z)$. Renormalizability requires that $Z_{\psi}^{-2}g$ and $Z_{\psi}^{-2}Z_{m}Z_{\psi}^{-1}g'$ are finite as $\Lambda \rightarrow \infty$; hence, $Z_u = Z_v Z_v^{1/2} Z_m^{-1/2}$. Requiring that $Z_u^4 Z_w \Gamma'_4$ be finite as $\Lambda \rightarrow \infty$ we then find, using the above considerations, that $Z_{\psi}^{4}Z_{\psi}Z_{m}\Gamma_{4}$ must remain finite as $\Lambda \rightarrow \infty$. Similar reasoning leads to the con-

FIG. 4. Graphs contributing to the self-energy Σ_n in the presence of an applied stress. Each cross represents a v_0^2 vertex.

FIG. 5. (a) Graphs contributing to the three-point vertex Γ_3 . (b) Graphs contributing to the four-point vertex Γ_4 .

clusion that $Z_{\psi}^3 Z_{\psi}^{1/2} Z_{m}^{3/2} \Gamma_3$ remain finite as $\Lambda \rightarrow \infty$.

With the above renormalizability assumptions on Γ_3 and Γ_4 we then find, using (A5) and (A6) that

$$
Z_w = 1 + \frac{5w_0}{64\pi} \ln \Lambda \tag{A7}
$$

APPENDIX B: RENORMALIZATION OF $G(\vec{x})$

Multiplicative renormalizability of the densitydensity correlation function

$$
G(\vec{x}) = \langle \exp\{iu_0[\psi(\vec{x}) - \psi(\vec{0})]\}\rangle
$$

implies the existence of a renormalization constant Z (independent of \vec{x}) such that $ZG(\vec{x})$ is finite when expressed in terms of the renormalized

FIG. 6. Graphs contributing to $G(\vec{x})$, the densitydensity correlation function. The wavy line represents $G_0(\vec{x})$.

parameters.

To zeroth order in w_0 ,

$$
G(\widetilde{\vec{x}}) = G_0(\widetilde{\vec{x}}) = \exp\{u_0^2[g_0(\widetilde{\vec{x}}) - g_0(\widetilde{\vec{0}})]\},\,
$$

where $g_0(\vec{x})$ is the Fourier transform of $g_0(\vec{k})$. Setting $\tilde{z} = 0$, for simplicity, we find

$$
g_0(\vec{x}_1, \tilde{z}=0) = (x_1 \Lambda)^{-u_0^2/(4\pi)}
$$
 (B1)

in agreement with Caille.

In $O(w_0)$ there are two classes of diagrams (Fig. 6) divergent as $\Lambda \rightarrow \infty$, evaluation of which yields

$$
G_a(\vec{x}_1, z=0) = -R'w_0u_0^4G_0(\vec{x})\ln\Lambda
$$
 (B2)

where R' is a positive nonuniversal coefficient. Thus, to first order in w_0 ,

$$
G(\widetilde{\vec{x}}) = \langle \exp\{iu_0[\psi(\widetilde{\vec{x}}) - \psi(\vec{0})]\}\rangle
$$
\n
$$
G(\vec{x}_1, z = 0) = (x_1\Lambda)^{-u_0^2/4\pi}(1 - R'w_0u_0^4\ln\Lambda)
$$
\n(B3)

whereupon

$$
Z = \Lambda^{u_0^2/4\pi} (1 + R' w_0 u_0^4 \ln \Lambda) \ . \tag{B4}
$$

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results, since the analogous approximation in the 2D XY model has been proven innocuous. See J. Toner, Ph.D. thesis, Harvard University, 1981 (unpublished).

- ¹³The spin-wave approximation neglects topological defects, namely, dislocation loops, which presumably play no role in determining the properties of the 1D solid, though they may be relevant to the description of the nematic —smectic-A transition. See D. R. Nelson and J. Toner, Phys. Rev. B 24, 363 (1981).
- 14 Using only the terms explicitly shown in (2.1) one concludes that $\lambda = (2q)^{-1}$. The higher-order terms represented by $O((\nabla^3 m)^2)$ in (2.1) would, however, result in $\lambda = (aq)^{-1}$ for some $a \neq 2$
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- When finite deformations are allowed as we have allowed here, two modes of description are available: the Lagrangian and the Eulerian. The former description employs the coordinates of a particle in its initial undeformed state as the independent variables, while the latter description employs the coordinates of the particle in its deformed state. For infinitesimal strains, the two descriptions are equivalent. For convenience, we use the Lagrangian viewpoint here, but our results are insensitive to this choice. [For a discussion of finite deformations, see, e.g., I. S. Sokolnikoff, Mathematical Theory of Elasticity (McGraw-Hill, New York, 1946), p. 28].
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- ¹⁸Note that k_z has the dimensions of (momentum)², and the renormalization of k_z is equivalent to the renormalization of m_0 in the unscaled variables u, \vec{x}_1 , and z.
- ¹⁹See Appendix A for details
- ²⁰The function h also depends on the dimensionless quantity $k_z^{1/2}/v_0$ but we consider the limit $k_z \rightarrow 0$ to obtain the elastic constant B^R at zero wave vector.
- We are indebted to A. P. Young for suggesting this calculation.
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- ²⁸The second sound measurements are not done at $k_1 = 0$, however, since the argument of the logarithm in (3.13) contains the combination $(k_z^2/\lambda^2) + k_\perp^4$ [where we have rescaled back to wave vectors measured in units of inverse length using (3.1)] the contribution from k_1 is negligible, unless $k_z = 0$.
- ²⁹Measurements by Delaye, Ref. 27, suggest that the smectic-A p-nonyloxy benzoate-p-butyloxy phenol has an unusually small λ , i.e., a relatively large w .
- See, e.g., B. Y. Cheng, B. K. Sarma, I. D. Calder, S. Bhattacharya, and J. B. Ketterson, Phys. Rev. Lett. 46, 828 (1981).
- 31 It seems very reasonable that B is higher in monolayer materials than in bilayer materials since presumably the two layers constituting a single bilayer can be squeezed together under compression. This degree of freedom is unavailable to monolayers. There does not, however, seem to be any particular reason that the undulational constant K_1 should significantly differ from bilayers to monolayers. We are grateful to S. Bhattacharya, R. Meyer, P. Pershan, and J. Toner for discussions of this point.