Emergent tilt order in Dirac polymer liquids

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We study a liquid of zigzagging two-dimensional directed polymers with bending rigidity, i.e., polymers whose conformations follow checkerboard paths. In the continuum limit the statistics of such polymers obey the Dirac equation for particles of imaginary mass. We exploit this observation to investigate a liquid of these polymers via a quantum many-fermion analogy. A self-consistent approximation predicts a phase of tilted order, in which the polymers may develop a preference to zig rather than zag. We compute the phase diagram and key response functions for the polymer liquid, and comment on the role played by fluctuations.

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Directed line liquids consist of quasi-one-dimensional objects that are preferentially oriented along a common direction about which they undergo thermal fluctuations [1–4]. Realizations include systems as diverse as polymer liquids under uniaxial tension [5–7], two-dimensional lamellar smectics [8], step edges on crystal surfaces [9], interfaces in the KPZ universality class [10], and vortex lines in planar type-II superconductors [11]. Quantum many-body physics provides powerful tools for analyzing the thermal equilibrium properties of classical systems of strongly interacting directed line liquids, by means of the well-known mapping between the configurations of classical directed lines in D-dimensional space and the world-lines of nonrelativistic quantum particles moving in \( D - 1 \) spatial dimensions [12, 13]. For example, in Refs. [11–13] this mapping has been used to relate the structure of non-intersecting, but otherwise non-interacting, two-dimensional directed polymer liquids to the properties of the non-interacting one-dimensional Fermi gas. As discussed in Ref. [10], the properties of three-dimensional directed polymer liquids follow from a mapping onto a two-dimensional system of fermions interacting via a Chern-Simons potential.

The two-dimensional directed polymers that we consider in the present Letter have an energetic preference to be straight, i.e., an energy cost to be bent. To date, by contrast, attention has primarily been focused on directed polymers that have an energetic preference to be short, i.e., an external tension controls the mean length. Unlike the Kratky-Porod [12] model, which features a curvature-based bending energy, the polymers in the current model bend only by a fixed angle. This model of zigzagging directed lines may also capture the effect of crystalline anisotropy in step edges on crystal surfaces. As we shall see, the appropriate quantum analog of the zigzagging directed line liquid consists of relativistic quantum particles, which, accordingly, are governed by the Dirac equation. This analogy, combined with a self-consistent field approximation, enables us to obtain information about local polymer density and alignment in the form of the mean values and correlations of these quantities. Inter alia, we shall also see that the interplay of bending rigidity and repulsive interactions leads to polymer alignment. This kind of interplay has long been known to promote striking collective phenomena, such as nematic [13] or smectic [8] ordering.

To identify the quantum analog appropriate to a single zigzagging directed line, we recall—following Feynman and Hibbs [14] (and further developments in Refs. [15–17])—that the (discretized) Feynman path-integral representation of the quantum propagator \( Z(C_f, C_i) \) between the initial state \( C_i \) and the final state \( C_f \) of a relativistic particle consists of a sum over zigzagging paths. For a particle of mass \( \mu \) taking a path with \( \tau \) turns, the amplitude is \((i\epsilon\mu)^\tau\) and the propagator is thus given by

\[
Z(C_f, C_i) = \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \sum_{\tau} (i\epsilon\mu)^\tau,
\]

where the sum is taken over all paths consistent with the initial and final states; \( \epsilon \) is the lattice constant, and we have chosen units such that \( \hbar = c = 1 \). The state \( C \) refers to the combination of the positional coordinate \( x \) of the particle and its motion direction \( \sigma \) (\( \equiv \pm \)). Passing to the continuum limit \( \epsilon \to 0 \), it has been shown [14] that for a particle evolving for a time \( L \), \( Z \) is given by the ma-
trix element \( \langle C_f | e^{-iL\hat{H}} | C_i \rangle \), where the \((1+1)\)-dimensional Dirac Hamiltonian \( \hat{H} \) is given in the Weyl representation, by \(-i\sigma_z \partial_x - \mu \sigma_x \), in which

\[
\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(2)

are the Pauli matrices, and the discrete degree of freedom is the direction of motion.

For a zigzagging directed line, the classical partition function \( Z(C_f, C_i) \) associated with the line statistics has a form similar to \( Z(C_f, C_i) \), i.e.,

\[
Z(C_f, C_i) = \frac{1}{2\pi} \sum (\epsilon \text{m})^2.
\]

(3)

Replacing \( i\mu \) by \( m \) in Eq. (1) transforms \( Z \) into \( Z \). Therefore, in the continuum limit we have that \( Z = \langle C_f | e^{-L\hat{H}} | C_i \rangle \), in which the imaginary-time Dirac Hamiltonian \( \hat{H} \) in the Weyl representation is given by

\[
\hat{H} = mI + \sigma_z \partial_x - m\sigma_x = \begin{pmatrix} \partial_x + m & -m \\ -m & -\partial_x + m \end{pmatrix}.
\]

(4)

For reasons that we shall discuss shortly, we have added to \( \hat{H} \) the trivial term \( mI \), where \( I \) is the identity. By analogy with the well-known equivalence between the Feynman path integral and time-dependent Schrödinger equation, we may analyze the statistics of the zigzagging directed line in terms of the time-dependent imaginary-mass Dirac equation

\[
-\partial_t \Psi = \hat{H} \Psi
\]

(5)

for the doublet \( \Psi \). We note that the Hamiltonian \( \hat{H} \) has been considered in Refs. [18, 19] in connection with polymer solutions. The orientation of a polymer segment (see Fig. 1), which we shall call its tilt, corresponds to the velocity of the quantum particle. It is associated with the operator \( dx/dl = [H, \hat{x}] = \sigma_z \). The thermal average of the polymer direction is therefore captured by the quantum expectation value \( \langle \sigma_z \rangle \).

To pass to the nonrelativistic (i.e., large-mass) limit of the imaginary-mass Dirac equation, we note that it reduces to a single second-order PDE—the telegrapher’s equation—which, combined with the continuity equation, \( \partial_t (\Psi_1 + \Psi_2) + \partial_x (\Psi_1 - \Psi_2) = 0 \), forms an equivalent description. Its solution is known [20], and captures a combination of diffusive and propagating (i.e., wave-like) motion. In the aforementioned limit, the telegrapher’s equation reduces to the diffusion equation \( \partial_t \Psi_{1,2} = (2m)^{-1} \partial_x^2 \Psi_{1,2} \) [20, 22], i.e., the quantum analog is governed by the (nonrelativistic) Schrödinger Hamiltonian \((2m)^{-1} \partial_x^2 \). To summarize, in the real-time nonrelativistic limit the Dirac equation becomes the Schrödinger equation, whereas in the imaginary-time nonrelativistic limit the telegrapher’s equation becomes the diffusion equation [17].

To analyze the many-polymer liquid, we make use of results for the one-polymer system, which follow from the separation-of-variables solution of the imaginary-mass Dirac equation. Thus, we hypothesize the separated solutions

\[
\Psi_{nk}(x; l) = \Re (\psi_{nk} e^{-iE_{nk} x} e^{ikx}),
\]

(6)

where \( k \) is the (real) momentum, and the eigenvalues \( E_{nk} \) and constant tilt-doublets \( \psi_{nk} \) may, in general, be complex. By inserting Eq. (6) into the imaginary-mass Dirac equation (5), we arrive at the reduced eigenproblem:

\[
\begin{pmatrix}
  ik + m - E_{nk} & -m \\
  -m & -ik + m - E_{nk}
\end{pmatrix}
\psi_{nk} = 0,
\]

(7)

which has nontrivial solutions provided \( E_{nk} = m \mp \sqrt{m^2 - k^2} \) (for \( n = 1, 2 \)). For \( k < m \), \( E_{nk} \) are real and the separated solutions have the form

\[
\Psi_{nk}(x; l) = (\Re \psi_{nk}) e^{-iE_{nk} x} \cos kx - (\Im \psi_{nk}) e^{-iE_{nk} x} \sin kx,
\]

whereas for \( k > m \) they have the distinct form

\[
\Psi_{nk}(x; l) = (\Re \psi_{nk}) e^{-im} \cos (kx \pm l\sqrt{k^2 - m^2}) - (\Im \psi_{nk}) e^{-im} \sin (kx \mp l\sqrt{k^2 - m^2}),
\]

(8)

resulting from \( E_{nk} \) being complex. The latter form results from the fact that the imaginary-mass Dirac Hamiltonian is non-Hermitian, and thus has both real and imaginary parts to its eigenvalue spectrum. Such a non-Hermitian Hamiltonian does not describe an isolated quantum system, although analogous Hamiltonians can be used to model certain open quantum systems [23].

Non-Hermitian Hamiltonians have also been applied to sheared directed line liquids under tension, via the mapping to a nonrelativistic quantum system subject to an imaginary vector potential [24–26]. When we come to study the response of zigzagging directed line liquids to shear stress, we shall—following Refs. [24, 26]—introduce the stress \( s \) coupled to the tilt operator \( \sigma_z \), so that \( H \rightarrow H + s \sigma_z \); equivalently, \( k \rightarrow k - is \), i.e., here, too, \( s \) serves as an imaginary vector potential.

We pause to mention a well-known simplification that holds for bulk properties of long systems, viz., ground-state dominance. Using bra-ket notation, a polymer segment localized at position \( x \) with tilt label \( \sigma \) corresponds to the quantum state \( |x\sigma\rangle \). We then define the eigenstates \( |nk\rangle = \int dx \sum \sigma \psi_{nk}(\sigma) e^{ikx} \), and express the transfer-matrix operator appearing in the partition function \( Z \) in the eigenstate basis as follows:

\[
e^{-L\hat{H}} = \sum_{n,k} |nk\rangle e^{-LE_{nk}} \langle nk| \approx |gs\rangle e^{-LE_{gs}} \langle gs|,
\]

(9)

where \( |gs\rangle \) denotes the eigenket for which \( \Re(E) \) is minimized. The series in Eq. (9) is indeed dominated (for large \( L \)) by a single ground state, provided the ground state is nondegenerate. By using the expression \( F = -T \ln Z \) for the thermodynamic free energy.
$F$ of the polymer system, together with Eq. (9), we obtain $F = TLE_{gs}$. For a single zigzagging directed line, the ground state is $(n,k) = (1,0)$, so that $E_{gs} = 0$ and $(\psi^{(+)}, \psi^{(-)}) = (1,1)/\sqrt{2}$.

Prior to giving our analysis of the many-polymer liquid, we note a simple, self-consistent variational argument for the many-body ground state energy $E_{gs}$ of the interacting liquid consisting of $N$ polymers at mean density $\rho$. As a consequence of thermal fluctuations, each polymer occupies a characteristic width $w$ in the $x$-direction. In analogy with work on lamellar smectics [8,27], we replace the interacting many-line system by a single line in a harmonic external potential. For the relativistic system, the Dirac oscillator [which is defined using a linear potential term, $V(x) = x\sigma_z$] is a solvable analog of the nonrelativistic harmonic oscillator [28–30]. Replacing the mass of the Dirac oscillator by an imaginary value, its energy eigenvalues acquire the form $E_{\lambda\mp} = m \pm \sqrt{m^2 - 2|\lambda\mp|w^2}$ (for positive integers $\lambda_-$ and nonnegative integers $\lambda_+$) [29,30]. Thus, given the lowest-energy state $\lambda_- = 1$ and the self-consistency condition $\rho = w^{-1}$, we conclude that

$$E_{gs}/N - E_{1-} = m - \sqrt{m^2 - 2\rho^2},$$

from which the polymer liquid free energy follows.

Returning to our main goal, we now formulate the statistical mechanics of the zigzagging directed polymer liquid in terms of quantum many-particle physics. To do this, we choose the polymers to be identical and indistinguishable. We focus on joint probability densities for the polymer segments that, in the quantum analogy, correspond to the real and positive subset of wavefunctions $\Psi(X;\Sigma)$ (where $X \equiv (x_1,\ldots,x_N)$, and $\Sigma \equiv (\sigma_1,\ldots,\sigma_N)$). Specifically, we consider a polymer liquid in which two segments that are tilted in the same direction cannot occupy the same location in space. Thus, two polymers cannot “comeove” but they may cross (see Fig. 1). For each crossing, we assign a statistical weight controlled by an interaction strength $v_0$. In the quantum analogy, this system corresponds to the sector of many-body quantum states that are symmetric under pairwise exchange of particles: $|x_1,x_2,\ldots;\sigma_1,\sigma_2,\ldots\rangle = |x_2,x_1,\ldots;\sigma_2,\sigma_1,\ldots\rangle$ etc., i.e., bosonic states, with the additional constraint that $|x_1,x_2,\ldots;\sigma_1,\sigma_1,\ldots\rangle = 0$ etc.

Within the quantum analogy, this system can be usefully addressed using Girardeau’s extension [31] of his 1D mapping [32] between hard-core bosons and noninteracting fermions. For a system possessing only spatial degrees of freedom [1,5,7] (i.e., without tilt), this mapping proceeds by using the factor $B(X) = \prod_{n < m} \text{sgn}(x_n - x_m)$ in the transformation $|X\rangle_B = B(X)|X\rangle_F$ between symmetric (boson, $B$) and antisymmetric (fermion, $F$) states. The Pauli principle, operative for the Fermi states, translates into a local hard-core repulsion for the Bose states, so that two bosons are excluded from occupying the same point in space [32]. This mapping may be extended to states with tilt, using $|X,\Sigma\rangle_B = B(X)|X,\Sigma\rangle_F$, i.e., by introducing a sign of $-1$ into the fermionic state under the exchange of the position (but not tilt) labels [31]. Thus, the bosonic state $|X,\Sigma\rangle_B$ indeed vanishes if $(x_i,\sigma_i) = (x_j,\sigma_j)$ for any pair of particles; but it need not vanish if $\sigma_i \neq \sigma_j$.

To explore structure in the polymer liquid, we now derive the corresponding quantum many-particle Hamiltonian in the occupation number representation. First, we define the states $|\{\sigma_{nk}\}\rangle_B = \prod_{nk} \langle \alpha_{nk} \rangle_a |0\rangle$, where $\alpha_{nk}$ are the particle occupation number of the states $|nk\rangle$, $c^\dagger_{nk}$ are the corresponding creation operators, and $|0\rangle$ is the no-particle state. As we are considering Fermi statistics, the operators $c^\dagger_{nk}$ obey anti-commutation relations. Using the eigenstates $\psi_{nk}(\sigma)$ of the single-particle Hamiltonian, we construct the field operators $\psi_{\sigma}(x) = \sum_{nk} \psi_{nk}(\sigma) e^{ikx} c_{nk}$, in terms of which the many-body Hamiltonian $\hat{H}$ has the form (c.f. Eq. 4)

$$\hat{H} = \int dx \left\{ \sum_{\sigma\sigma'} \hat{\psi}_{\sigma}^\dagger \hat{H}_{\sigma\sigma'} \hat{\psi}_{\sigma'} + v_0 \hat{\psi}_{\sigma}^\dagger \hat{\psi}_{\sigma} \right\},$$

where all of the field operators have argument $x$. Next, by analogy with quantum statistical mechanics, we introduce $l$-dependent operators $\hat{\psi}_{\sigma}(x; l) \equiv e^{ilx} \hat{\psi}_{\sigma}(x) e^{-ilx}$ and the partition function $Z = \text{Tr} e^{-\hat{H}l}$ (where the trace $\text{Tr}$ is taken over all $N$-particle states), and thermal expectation values of operators $\hat{O}$ are given by $Z^{-1} \text{Tr} \hat{O} e^{-\hat{H}l}$.

Thus, the zigzagging polymer liquid maps to an interacting $N$-fermion fluid described by the Hamiltonian [14]. For the case $v_0 = 0$, the exact ground state of this Fermi fluid has only the $N$ lowest-energy single-particle states occupied. The nature of this ground state changes qualitatively as the value of the Fermi wavevector $k_F$ (which is related to the density via $\rho = k_F/\pi$) is increased to $m$. For $k_F < m$, the Fermi sea fills the bottom portion of the spectrum and the real part of the total
energy is given by $\Re E = mN - \sum_{k<k_F} \sqrt{m^2 - k^2}$ (see Fig. 2). For $k_F > m$, there are many degenerate ground states, all with $\Re E = mN - \sum_{k<m} \sqrt{m^2 - k^2}$; in these states all single-particle states with $n=1$ and $k < m$ are occupied, with the rest of the occupied states being arbitrarily chosen from the doubly-degenerate band that has $\Re E = m$ and $k > m$ (see Fig. 2). For $k_F > m$, a unique ground state can be achieved by imposing a shear stress $\sigma$ (see Fig. 2). Thus, for $\sigma \neq 0$, the ground state is non-degenerate for any particle density.

Using these fermion ground states, we calculate the correlations of density and tilt in the zigzagging directed line liquid with $v_0 = 0$ using the exact expression

$$\langle \hat{\rho}(q, \omega) \hat{\rho}(-q, -\omega) \rangle = \Re \sum_{knk'} \frac{O_{n(k+q)} - \bar{O}_{n'k}}{E_{n(k+q)} - E_{n'k} - \omega},$$

where $\hat{\rho}$ is an operator (e.g., $\hat{\rho} \equiv \sum_a \hat{\psi}_a^\dagger \hat{\psi}_a$ or $\hat{\zeta} \equiv \sum_{ab} \hat{\psi}_a^\dagger (\sigma_z)_{ab} \hat{\psi}_b$), $O_{nk}$ is the expectation value of $\hat{O}$ in the single-particle state $nk$. We compute these correlation functions using the complex basis (6). For $\omega = 0$, the results are plotted in Fig. 3.

Next, we study the uniform tilt susceptibility in analogy with the Stoner theory of itinerant magnetism, which addresses a repulsive spin-1/2 Fermi gas [34]. To do so, we use a self-consistent approximation and ignore fluctuations, which we recognize destroy true long-range order in one-dimensional Fermi systems—instead, we expect the true ground state to have long-range tilt correlations. For zigzagging directed lines, the self-consistent equation (SCE) results from the Hartree-Fock approximation of the interaction: $v_0 (\psi_-^\dagger \psi_- + \psi_+^\dagger \psi_+) + v_0 (\psi_-^\dagger \psi_+ + \psi_+^\dagger \psi_-)$. Rewriting this expression in terms of the expectation value $\langle \hat{\zeta} \rangle$, the relevant term becomes $-s_{sc} \hat{\zeta}$, where

$$s_{sc} = \frac{v_0}{2} \langle \hat{\zeta} \rangle,$$

which is the SCE. We evaluate $\langle \hat{\zeta} \rangle$ in the ground state by using a (nonorthogonal) transformation to the eigenbasis of the Hamiltonian [33] to obtain

$$\langle \hat{\zeta} \rangle = \frac{1}{\pi} \Im \left( \sqrt{m^2 - (k_F + i s_{sc})^2} \right).$$

Substituting this expression into the SCE (12), we find a non-trivial solution if and only if $(1+g^2)k_F^2 > m^2$, where $g \equiv v_0/2\pi$ (see Fig. 4). In this region, the SCE (with its neglect of fluctuations) predicts a tilt of the polymer system in equilibrium (see Fig. 4). Note that for $k_F > m$, this solution exists even for the case $v_0 = 0$; this results from the fact that an applied stress $s$ breaks the degeneracy between the two bands, as shown in Fig. 2(a), leading to polymer-system tilt that increases with density beyond $m/\pi$. The critical line shown in Fig. 4 corresponds to an Ising-like continuous phase transition in the mean-field approximation. Accordingly: (i) the Ising order parameter (i.e., the tilt) scales as the square root of the distance to the critical line, $\langle \hat{\zeta} \rangle = \pi^{-1} \sqrt{k_F^2 - m^2(1+g^2)^{-1}}$; (ii) on the critical line, the tilt scales with the shear stress as $\langle \hat{\zeta} \rangle \sim \frac{1}{\pi} \left( \frac{2m^2}{1+g^2} \right)^{1/3} s^{1/3}$; and (iii) the uniform tilt susceptibility diverges on approach to the critical line (see Fig. 4), as seen in the expression

$$\chi = \left\{ \begin{array}{ll}
\frac{1}{\pi} \frac{k_F}{\sqrt{m^2 - k_F^2 - gk_F}} & \text{for } \langle \hat{\zeta} \rangle = 0; \\
\frac{1}{\pi} \frac{m^2 g}{1 + g^2 (1+g^2)k_F^2 - m^2} & \text{for } \langle \hat{\zeta} \rangle \neq 0.
\end{array} \right.$$
We note that the model described here addresses the structure of the zigzagging polymer liquid on mesoscopic length scales, i.e., between the molecular structure of the polymer fluid and its larger-scale collective properties. We also note that Eq. (11) is a variant of the Thirring model [36]. As is well known, the original Thirring model can be solved exactly by using a mapping onto the bosonic sine-Gordon model [37]. However, using the same bosonization methods, the Hamiltonian (11) does not map onto a realizable Hamiltonian for a Bose system because the one-particle energy, Eq. (4), maps onto a complex term. Thus, it remains an open question whether the many-body problem analyzed here is exactly solvable.

We close with some comments on the role of dimensionality. (i) It would be interesting to explore whether extensions of the Hamiltonian (11) could be applied to higher-dimensional systems of directed lines. (ii) Although possible [3], the transmutation of quantum statistics in higher-dimensional systems requires a more elaborate construction. (iii) In two-dimensional directed polymer liquids, fluctuations eliminate true long-range order, though vestiges of it remain in the form of long-range correlations.

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and substituting the SCE into Eq. (11) to obtain an expression for the mean-field free energy of zigzagging directed lines, which we then minimize w.r.t. $s_{ss}$.