Attractive Inverse Square Potential, $U(1)$ Gauge, and Winding Transitions

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(Received 20 October 2013; published 20 February 2014)

The inverse square potential arises in a variety of different quantum phenomena, yet notoriously it must be handled with care: it suffers from pathologies rooted in the mathematical foundations of quantum mechanics. We show that its recently studied conformality breaking corresponds to an infinitely smooth winding-unwinding topological transition for the classical statistical mechanics of a one-dimensional system: this describes the tangling or untangling of floppy polymers under a biasing torque. When the ratio between torque and temperature exceeds a critical value the polymer undergoes tangled oscillations, with an extensive winding number. At lower torque or higher temperature the winding number per unit length is zero. Approaching criticality, the correlation length of the order parameter—the extensive winding number—follows a Kosterlitz-Thouless-type law. The model is described by the Wilson line of a $(0+1)$ $U(1)$ gauge theory, and applies to the tangling or untangling of floppy polymers and to the winding or diffusing kinetics in diffusion-convection reactions.

DOI: 10.1103/PhysRevLett.112.070401 PACS numbers: 03.65.Vf, 11.15.-q, 64.70.Nd, 87.15.Zg

The quantum mechanics of the inverse square potential (ISP) [1,2] is an old problem that has attracted much recent attention [3–10]. It is relevant to phenomena as diverse as the Efimov effect for short range interacting bosons [11,12] (recently confirmed experimentally [13]), the interaction between an electron and a polar neutral molecule [14,15], the near-horizon problem for certain black holes [16,17], the anti–de Sitter/conformal field theory correspondence [18], and nanoscale optical devices [19]. In statistical mechanics, the inverse square potential represents the borderline case for a phase transition for the long-ranged 1-D Ising model [20–23].

While the mathematics of the ISP is well understood [1,2], its practical use remains often problematic [3–10]. The quantum mechanics of its conformally invariant Hamiltonian is well posed for repulsive or weakly attractive couplings, yet it is not self-adjoint for strong attractions [24–26], leading to unphysical pathologies typical of singular potentials [27]. Most relevantly, its bound spectrum is a continuum and unlimited from below [1,2]. The problem is often rendered physical by a short-distance cutoff, when possible, or by other renormalizations [3,8]: in all cases conformality is lost either by regularization or by a renormalization anomaly.

When regularized by a finite cutoff, the potential produces an infinite but discrete and limited spectrum of bound states and negative energies, with a defined ground state. At the crossover between strong and weak attraction the bound states disappear in the same fashion as the inverse correlation length in the Kosterlitz-Thouless (KT) transition [28], a feature of loss of conformality [6]. This is suggestive of an associated (topological) transition.

Here we show that the problem can indeed be related to an infinitely smooth topological transition for a one-dimensional system that is biased to wind around the pole of a non-simply-connected space. The order parameter, as we shall see, is then the average winding number, which approaches zero infinitely smoothly at the transition while its correlation length follows a KT law. The transition is thus between the winding and nonwinding functional submanifolds of the Hamiltonian, which can be made topologically distinct by boundary conditions. The removal of these boundary constraints at the transition corresponds to the extension of the gauge space for a $(0+1)$ $U(1)$ symmetry, whose Wilson line describes our system.

For physical definitiveness, the model can describe a tangling or untangling phase transition for floppy polymers [29–31] under torque: current single molecule manipulation techniques [32] could test it experimentally. Not surprisingly, it is also associated with a kinetic transition for a diffusion-convection reaction in a screw dislocation.

Consider first the one-dimensional "Hamiltonian" for the attractive ISP

$$\hat{H} = -\frac{1}{2\chi}\left(\frac{d^2}{d\rho^2} + \frac{\gamma^2}{\rho^2}\right), \tag{1}$$

which can be made self-adjoint for $|\gamma| > 1/2$ by a short distance cutoff $\rho \geq \bar{\rho}$ such that Eq. (1) acts on smooth functions of $[\bar{\rho}, \infty)$ with a Dirichlet (zero) boundary condition at $\bar{\rho}$ [3]. We associate to it the partition function (or density operator)

$$Z_\gamma(\rho_l, \rho_0) = \int_{\rho(0)=\rho_0, \rho>\bar{\rho}}^{\rho(l)=\rho_l} [d\rho] \exp\left[-\int_0^l \left(\frac{\chi}{2}\dot{\rho}^2 - \frac{\gamma^2}{2\chi\rho^2}\right) ds\right], \tag{2}$$

such that (with the above regularization for $\hat{H}$) [33]

$$Z_\gamma(\rho_l, \rho_0) \propto \langle \rho_l | e^{-l\hat{H}} | \rho_0 \rangle. \quad (3)$$

(Equipartition factors in χ, irrelevant to the transition, are neglected in the following.) We then introduce

$$\langle \omega \rangle = l^{-1} \partial_\gamma \ln Z_\gamma = \langle k^{-1} \rangle \gamma \quad (4)$$

as an order parameter. The second equality in Eq. (4) defines the average winding compliance $\langle k^{-1} \rangle$, the reciprocal of a generalized rigidity. Equation (4) can be rewritten as $\langle k^{-1} \rangle = 2l^{-1} \partial_{\gamma^2} \ln Z$, and then from Eq. (2) we find

$$\langle k^{-1} \rangle = \langle 1/\chi\rho^2 \rangle. \quad (5)$$

As we will see below, as $\gamma \to (1/2)^+$ the order parameter $\langle \omega \rangle$ disappears in the thermodynamic limit ($l \to \infty$) and thus the generalized rigidity diverges.

The physical meaning of the above treatment becomes clearer by performing a Hubbard-Stratonovich transformation on Eq. (2) in the auxiliary variable ω, which yields

$$Z_\gamma(\rho_l, \rho_0) \propto \int_{\rho(0)=\rho_0, \rho>\bar{\rho}}^{\rho(l)=\rho_l} [\rho d\omega d\rho] \exp\left(-\beta \int_0^l \mathcal{H} ds\right) \quad (6)$$

for the energy per unit length $\mathcal{H}$, given by

$$\beta\mathcal{H} = \chi(\dot{\rho}^2 + \rho^2\omega^2)/2 - \gamma\omega. \quad (7)$$

(Here $\beta = 1/T$; the Boltzmann constant is taken to be $k_B = 1$). Note that, as a consequence of the transformation, there are no boundary conditions on ω.

The ρ in the functional measure $[\rho d\omega d\rho]$ is due to the inverse Gaussian integration over ω and the functional measure is thus reminiscent of a surface element in polar coordinates. Indeed Eqs. (6) and (7) control the statistical mechanics of a field $\psi(s) = \rho(s) \exp[i \int^s \omega(s') ds']$, which describes trajectories in a punctured (because $\rho > \bar{\rho}$) complex plane. Then, from Eq. (7), the order parameter $\langle \omega \rangle$ in Eq. (4) is simply the average linear density of the winding number (up to a factor 2π) of these trajectories around the pole: the quantum-mechanics of the ISP with an ultraviolet cutoff is thus turned into the statistical mechanics of a one-dimensional object winding around the pole of a non-simply-connected plane.

For a system described by this model (see the conclusion for more realizations) consider a floppy polymer—a random chain [31,33] of length l—made of $N = l/a$ monomers of length a, held under tension f and subjected to a torque Γ by magnetic or optical tweezers [32], as in Fig. 1. In a continuum limit, $\psi(s)$ represents the deviation from the straight filament configuration in the perpendicular plane and s is the intrinsic coordinate. The contribution from tension to the energy density per unit length, neglecting subdominant terms, is $-f dh/ds = f\dot{\psi}^*\dot{\psi}/2 = f(\dot{\rho}^2 + \rho^2\omega^2)/2$. Here dh is the experimentally measured change in distance h between beads (Fig. 1). The simple connectedness of the space (and thus of the plane orthogonal to the experimental apparatus) is removed by considering another polymer, held straight, around which our polymer can tangle (Fig. 1). Then the energy contribution to the torque is $-\Gamma \int_0^l \omega ds$ as $\int_0^l \omega ds$ is the mutual angular deviation between the beads on which the torque acts. There are boundary conditions $\rho(l) = \rho(0) = \rho_0 > \bar{\rho}$ at the extremes, but clearly not on the angular variable. Such a system is described by the energy in Eq. (7) if $\chi = f/T$, $\gamma = \Gamma/T$. One might also consider two identical polymers, described by ϕ_1, ϕ_2, and then $2\psi = \phi_1 - \phi_2$ (the "center of mass" coordinate $\phi_1 + \phi_2$ only contributing equipartition). In both cases $\bar{\rho}$ is the average of the two radii. This problem of biased tangling can be extended beyond the experimental setting, for instance to the case of a floppy polymer tangling around another polymer with large persistence length (e.g., ssDNA tangling around helical DNA).

We now analyze the transition, which corresponds to the disappearance of the extensive winding of the two polymers. In the thermodynamic limit of large l, Eq. (3) projects

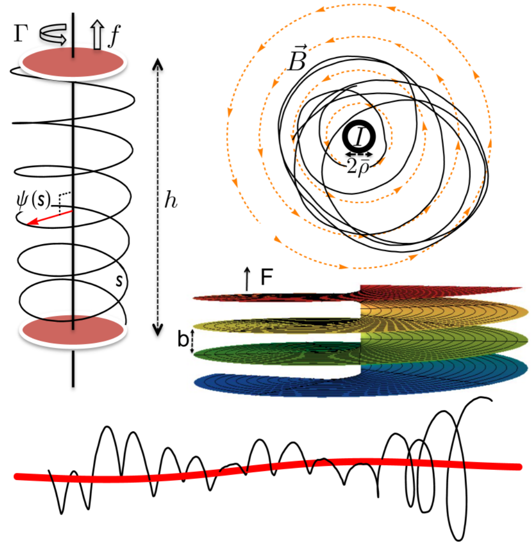

FIG. 1 (color online). Left: schematics of a possible experimental setting; a fluctuating polymer, here in a helical configuration, is held at its ends with a tension f between beads at distance h, subject to a torque Γ, tangling around the straight polymer at the center, and is described by the two-dimensional vector $\psi(s)$ (red arrow) in the plane perpendicular to h, while s is the intrinsic coordinate. Top right: a random chain with magnetized monomers of magnetic moment parallel to the tangent curling around a current I generating a magnetic field $\vec{B}$. Middle right: the convection-diffusion-reaction (of dopant tracers) takes place on a Riemann surface (a screw dislocation) while the angular drift is provided by the applied field F along the z direction; b is the Burgers vector. Bottom: a floppy polymer biased to tangle around a polymer of larger persistence length.

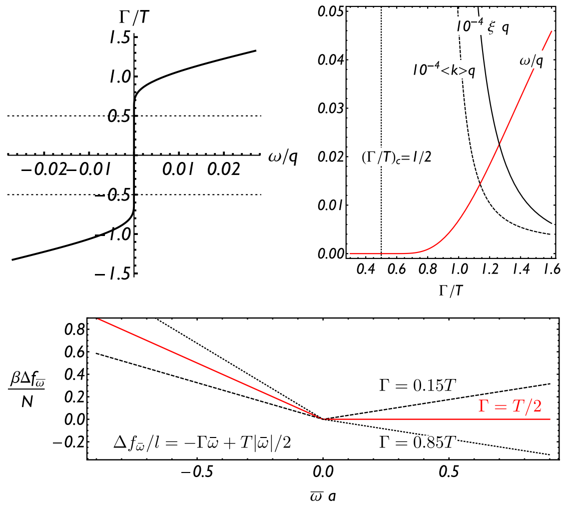

FIG. 2 (color online). Left: The transition in the $\gamma = \Gamma/T$ vs ω plot; $|\Gamma/T| \to 1/2$ as $\omega \to 0$. Right: as $\Gamma/T \to 1/2+$ the average helicity $\langle\omega\rangle$ (red solid line) tends to zero exponentially fast, while both the generalized helical rigidity $\langle k\rangle \equiv 1/\langle k^{-1}\rangle$ (dashed black line) and the correlation length ξ (black solid line) approach infinity with exponential behavior. Bottom: the free energy density contributed by a definite helicity $\bar\omega$ from the heuristic argument in Eq. (12); for $\gamma < 1/2$ we always have an increase of free energy, whereas at criticality ($\gamma = 1/2$) all ω of the same sign of γ are admitted; for $\gamma > 1/2$ the largest possible winding ω (defined by cutoff) provides the smallest lowering of the free energy.

onto the lowest bound state of eigenvalue ϵ_0—if there is one—giving $\langle\omega\rangle = -T\partial_\gamma\epsilon_0 \neq 0$. The discrete spectrum of the operator in Eq. (1) is known to disappear when $|\gamma| < 1/2$, pointing to a transition at $T_c = 2|\Gamma|$. For $T > T_c$ the contribution from the continuum spectrum in Eq. (3) is nonextensive in l, and the partition function effectively reduces to equipartition, or $Z \propto \chi^{-l/a}$, independent of γ, and thus $\langle\omega\rangle = 0$: above the transition the extensive helical structure is lost [34].

When $T \to 2\Gamma^-$, the 1-D Schrödinger problem of Eq. (1) on a half line with a cutoff is well studied [3]. Defining $\nu^2 = \gamma^2 - 1/4$, the disappearing lowest bound eigenvalue can be approximated in the limit $\nu \to 0^+$ [3] as

$$\epsilon_0 = -qe^{-\frac{2\pi}{\nu}}[1 + O(\nu)], \tag{8}$$

with $q^{-1} = 3.17(2\ldots)\bar\rho^2\chi/T$. From Eqs. (4) and (8) it follows that the helical order parameter disappears at the transition with infinite smoothness (Fig. 2) as

$$\langle\omega\rangle \simeq 2\,\pi q\gamma\nu^{-3}e^{-\frac{2\pi}{\nu}}[1 + O(\nu^2)] \tag{9}$$

and the transition is therefore of infinite order, as expected given its topological nature. The generalized rigidity $\gamma/\langle\omega\rangle$ approaches infinity exponentially fast at the transition and, therefore, from Eq. (5), so does $\langle\rho^2\rangle$.

From the statics of Eq. (7) we can gain some insight into the transition. The local minima of $\mathcal{H}$ (for variations at fixed boundaries) are uniform trajectories, or $\dot\psi(s) = 0$, corresponding to a straight polymer parallel to the experimental axis (its statistical mechanics corresponds to planar oscillations). However, for $\gamma \neq 0$, winding trajectories, which are not stationary points of the functional (in the sense that $\delta\mathcal{H}/\delta\psi \neq 0$), have lower energy. Among these, if ρ is constrained, the global minimum is a uniform helix with

$$\omega = k(\rho)^{-1}\gamma = \frac{\gamma}{\chi\rho^2}, \tag{10}$$

where $k(\rho)$ is the linear density of helical rigidity per unit length and, therefore, k^{-1} is the static helical compliance introduced in Eq. (5). Note that the generalized winding compliance of Eq. (5) is simply the thermal average of the static compliance Eq. (10). The energy of the helix is then

$$\beta V(\rho) = -\frac{\gamma^2}{2\chi\rho^2}. \tag{11}$$

The cutoff provides a lower bound for the energy at $\rho = \bar\rho$ and helicity $\omega_0 = k(\bar\rho)^{-1}\gamma$.

The global minimum of the regularized functional $\mathcal{H}$ in Eq. (7) corresponds to a uniform winding around the pole, while its excitations are straight polymers. These two classes of trajectories are topologically distinct in the non-simply-connected plane and a transition can happen when their free energies become degenerate. Indeed entropy reduction is the cost of structure: winding trajectories, although favored by energy, are entropically disadvantageous compared to the nonwinding ones: this competition drives the transition and suggests the heuristic argument below.

Summing over fluctuations in ρ only, while maintaining $\bar\omega$ fixed, we obtain the partition function of a helix of uniform winding angle $\bar\omega$, or $Z_{\bar\omega} = e^{\gamma\bar\omega l}\int[d\rho]\exp[-\frac{\chi}{2}\int_0^l(\dot\rho^2 + \rho^2\bar\omega^2)ds]$. The latter is a harmonic problem in ρ when $\bar\omega \neq 0$, while for $\bar\omega = 0$ it reduces to free oscillations and thus equipartition $Z_{\bar\omega} \propto \chi^{-l/a}$. For large l we can project on the lowest eigenvalue $|\bar\omega|/2$. By subtracting the equipartition free energy density $(\ln\chi)/2a$ (obtained for $\bar\omega = 0$) from the free energy density $f_{\bar\omega} = -Tl^{-1}\ln Z_{\bar\omega}$, one arrives at the (linear density of) free energy difference contributed by the helicity $\bar\omega$:

$$\Delta f_{\bar\omega} = -\Gamma\bar\omega + T|\bar\omega|/2. \tag{12}$$

Equation (12) implies that both energy $-\Gamma\bar\omega$ and entropy $\Delta s = -|\bar\omega|/2$ are reduced by a winding trajectory. As expected, their interplay drives the transition: for $|\gamma| < 1/2$, helical structures are suppressed, as any helicity $\bar\omega \neq 0$ increases the free energy. However, when $|\gamma| > 1/2$, the entropic cost of winding can be offset by an energetic gain, and helical structures of the same orientation of Γ lower the free energy (Fig. 2) [35]. As with the KT transition, the heuristic, entropic argument correctly predicts the critical temperature ($T_c = 2|\Gamma|$).

Interestingly, the heuristic result in Eq. (12) is exact at the transition with the substitution $\bar{\omega} \to \langle\omega\rangle$. In fact, from $f = T\epsilon_0$, $s = -\partial_T f$, and Eq. (8), we obtain

$$\Delta s = -\frac{1}{2}\langle\omega\rangle[1 + 2\nu^2 + O(\nu^3)]. \tag{13}$$

Since the heuristic computation is based on a uniform winding angle, its exactness at the transition suggests that the order parameter tends to uniformity at criticality. As it disappears, its fluctuations must then tend to zero, while their correlation length must approach infinity. The first statement is proved true by differentiating the expression for $\langle\omega\rangle$ in Eq. (9) with respect to γ. We establish the second one below.

Correlation lengths can be computed by introducing a varying external field $\gamma(s) = \gamma + \eta(s)$ with γ uniform, as before. The winding correlation function $G(s_1, s_2) = \langle\omega(s_1)\omega(s_2)\rangle - \langle\omega\rangle^2$ is given by [36]

$$G(s_1, s_2) = \frac{\delta^2 \ln Z[\eta]}{\delta\eta(s_1)\delta\eta(s_2)}\bigg|_{\eta=0}, \tag{14}$$

where the new partition function $Z[\eta]$ is still given by Eq. (3), with the replacement $l\hat{H} \to l\hat{H} + \gamma\int_0^l [\eta(s)/\chi\rho^2]ds$. Standard perturbation calculations in imaginary time s yield, for large $|s_1 - s_2|$,

$$G(s_1, s_2) \propto e^{(\epsilon_0 - \epsilon_1)|s_1 - s_2|}. \tag{15}$$

From Eqs. (15) and (9) we have for the correlation length

$$\xi = -(\epsilon_0 - \epsilon_1)^{-1} \sim \exp\frac{2\pi}{\sqrt{\gamma^2 - 1/4}} \tag{16}$$

[since $\epsilon_1/\epsilon_0 \sim \exp(-4\pi/\nu)$ at the transition [3]]. Equation (16) is the same result of the KT model (but with Γ replacing T). This can be expected as both transitions are topological in nature and both coincide with the breaking of conformality [6]. However, unlike the KT case, an external field Γ breaks the symmetry of our problem and provides an order parameter $\langle\omega\rangle$.

Our analysis also provides a clear topological explanation for the well known anomalous symmetry breaking of the ISP via renormalization [3,5–7]. The transition corresponds to tangled fluctuations contributing to the partition function below the transition, and untangled above. These trajectories are topologically distinct in the punctured space. Taking the cutoff $\bar{\rho} \to 0$ does not restore simple connectedness. Indeed the limit can be taken together with $\gamma \to (1/2)^+$ in such a way that $\langle\omega\rangle$ in Eq. (9) remains finite, or that ε_0 in Eq. (8), remains finite, which corresponds to the quantum anomaly of the ISP in Eq. (1).

Finally, we show that the model corresponds to the theory for the Wilson line of the (nondynamical) $U(1)$ gauge theory in $(0+1)$ dimensions for a field $\phi = \rho \exp i\alpha$:

$$\beta\mathcal{L}_{\phi,A} = \chi|(\partial_s - iA)\phi|^2/2 + \zeta A, \tag{17}$$

which is invariant under $\phi \to \phi \exp i\Lambda$, $A \to A + \partial_s\Lambda$, if Λ has periodic boundary conditions, $\Lambda(s) = \Lambda(0)$, and thus cannot change the total winding number for ϕ. Then our previous coordinate ψ can be considered as the Wilson line of the gauge theory (17) in ϕ and A:

$$\psi(s) = \phi(s)e^{-i\int^s A(t)dt}. \tag{18}$$

From Eq. (18), our winding parameter $\omega = \partial_s\alpha - A$ is the relevant coordinate, mapping a gauge-invariant functional manifold orthogonal to the gauge lines. Conversely, the new coordinate $\eta = \partial_s\alpha + A$ describes the gauge trajectories: indeed η flows with the gauge as 2Λ.

With this in mind Eq. (17) can be rewritten as

$$\beta\mathcal{L}_{\phi,A} = \chi(\dot{\rho}^2 + \rho^2\omega^2)/2 - \zeta(\omega - \eta)/2, \tag{19}$$

since $2A = \eta - \omega$. In the partition function the term $\zeta\eta/2$ factors into the irrelevant integration over the gauge trajectories (while the Faddeev-Popov determinant is inconsequential, the theory being Abelian), and we are effectively left with $\beta\mathcal{L}_{\phi,A} = \beta\mathcal{H}_\psi$, our energy for ψ given by Eq. (7), but with $\gamma = \zeta/2$.

We see now that the transition in the $U(1)$ gauge theory corresponds to $\zeta = 1$, for which the expression $\exp(i\zeta\int^s Adt)$ becomes invariant toward a gauge with free boundaries in the thermodynamic limit. Indeed the allowed values $\Lambda(s) - \Lambda(0) = 2\pi n$ correspond to the change of winding number per unit length $2\pi n/l$ which approaches continuum as $l \to \infty$. At the transition the gauge space extends to transformations that can change the average winding number of the field: that is natural, as the two functional spaces (winding and unwinding trajectories) are only topologically distinct at fixed boundaries, a constraint removed at the transition.

Before concluding, we propose other realizations. Considering ψ as a two-dimensional vector $\vec{x}$ we write Eq. (7) as

$$\beta\mathcal{H} = \chi|\dot{\vec{x}}|^2/2 - \gamma\dot{\vec{x}}\cdot\vec{w}(x), \tag{20}$$

where $\vec{w} = \vec{\nabla}\theta(\vec{x}) = \hat{e}_3\wedge\hat{x}/|\vec{x}|$ is the field of an elementary vortex ($\hat{e}_3$ is the unit vector perpendicular to the plane, $\theta(\vec{x})$ the angular coordinate of $\vec{x}$). If $\gamma\vec{w}$ represents a magnetic field generated by a current I perpendicular to the plane, the path integral in Eq. (6) describes the probability distribution for a magnetized ideal random chain [33] in the magnetic field, where each monomer has a magnetic moment $\vec{m} \propto d\vec{x}$ and $\gamma = \mu_0 |m| I / 2\pi T$ ($\chi = 2/a$).

Finally, if $l \to t$, $\chi = 1/2D$, where D is the diffusivity, and if $\{(\vec{x}_0, t_0) \to (\vec{x}, t)\}$ are chosen as boundary conditions for the trajectories in the path integral then, from Eqs. (6) and (20) , $P(\vec{x}, t; \vec{x}_0, t_0) \propto Z$ describes the solution of the following convection-diffusion-reaction equation

$$D^{-1}\dot{P} = \vec{\nabla} \cdot (\vec{\nabla} P - \gamma \vec{w} P) + P\gamma^2 w^2/4 \qquad (21)$$

on a helical Riemann surface under drift $D\gamma\vec{w}$. The Riemann surface can be a screw dislocation in a material where only in-plane diffusion is allowed [37]. Then drift can come from a field $F\hat{e}_3$ parallel to the Burgers vector $\vec{b} = \hat{e}_3 b$ (Fig. 1), since $z/b = \theta/2\pi$. Then $\gamma = 2\mu F b/D$, where μ is the mobility ($2\mu F b$ is the vorticity of the drift): the transition corresponds to a competition between diffusivity and drift. A nonzero order parameter in Eq. (4) implies a uniform (in time) climbing of the dislocation, or $z \sim h\theta/2\pi \sim h\langle\omega\rangle t/2\pi$.

In conclusion we have reported a topological winding or unwinding transition connected with the quantum loss of conformality of the attractive ISP. The quantum anomaly of the potential at strong couplings is related to the non— simple connectedness of the manifold that allows for topological distinction. Below the transition winding topologies are energetically favored, although entropically unfavored, and vice versa above the transition. We have proposed possible physical applications including polymer physics and diffusion-convection reactions. In particular, an experiment in single molecule manipulation of an appropriate floppy polymer (Fig. 1) could reveal the transition: at room temperature the critical torque is ~2pN × nm.

C. N. is grateful to P. Lammert for discussions. This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DEAC52-06NA25396.

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