The quantum character of elastic instabilities in worm-like chains

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A formal mapping is carried out between elastic instabilities undergone by inextensible filaments in 2d, and nonrelativistic, time-independent quantum mechanics in 1d (with restrictions on relative phase differences). Three simple and physically realizable applications of the mapping are given in detail; the quantum counterparts of these are particle in a box, particle in a delta-function well, and particle in a triangular well. Finite temperature considerations in the first application reveal a connection between the persistence length of the elastic filament and the thermal de Broglie wavelength of the ideal gas. The third application involves a novel variant of the “self-buckling” problem. Finally, the mapping is used to see what a many-body problem (in the Hartree approximation) looks like when recast as an elastic instability problem.

Energy quantization, normalization, and observable consequences of relative phase differences are usually regarded as concepts belonging to the realm of quantum mechanics. Yet these same concepts also apply to elastic instabilities in thin rods, the theory of which dates back to the days of Euler but is not widely known to physicists working outside of soft matter. Several prior analogies have been made between rod and plate buckling problems and quantum mechanical problems [1][6], but a general and unifying framework is absent. In some of the above works, the wavefunction-like entity is said to be the shape (deflection) of the buckled rod [1][2][6], in others the slope (tangent vector) of the rod [3][4], and yet in another the curvature of the rod [5]. All place restrictions on the form of the potential energy-like entity, it being either a constant [1][2][6], or of a harmonic oscillator form [3][4], or a symmetric function with respect to the midpoint of the rod [5]. Here we present a formal mapping between elastic instabilities in 2d and time-independent quantum mechanics in 1d that is considerably more general than those analogies suggested before. We find that if the wavefunction-like entity is taken to be the slope of the rod, then the normalization condition maps directly to an inextensibility constraint for the rod, and the potential energy function maps to an arbitrary body force acting parallel to the rod.

Let us start by briefly reviewing deformations of rods [7]. An elastic rod can deform by bending, by stretching or compressing lengthwise, and by torsion, while still remaining a rod. We will specialize to rods with small deformations confined to a plane, i.e., rods in 2d, and ignore torsion. If such a rod is oriented along \( \hat{x} \), with transverse deflection \( u(x) \) much smaller than the rod’s length, and axial strain \( d\ell(x)/dx \ll 1 \), the deformation energy of the rod is given by

\[
H = \frac{\kappa}{2} \int dx \left( \frac{du}{dx} \right)^2 + \frac{\mu}{2} \int dx \left( \frac{d\ell}{dx} \right)^2.
\]

(1)

Here \( \kappa \) is called the bending modulus and \( \mu \) is called the stretching modulus. These scale as \( A^2Y \) and \( AY \) respectively, where \( Y \) is Young’s modulus and \( A \) is the cross sectional area. Thus if the rod is very thin, \( \kappa \ll \mu \), meaning the rod’s resistance to stretching and compressing is much greater than its resistance to bending. Biopolymers, carbon nanotubes, and certain other filamentous molecules having \( \kappa \ll \mu \) are often modeled by removing the second term in Equation (1) and replacing it with an inextensibility constraint. This is the essence of the so-called “worm like chain” (WLC) model [8][10]. In what follows, we will use the concept of a “WLC limit,” which we define as Equation (1) combined with the limit \( \kappa/\mu \to 0 \).

Suppose the rod is subjected to longitudinal contact and/or body forces \( T(x)\hat{x} \), but no transverse forces. If the rod is in equilibrium, any small section of it must obey the equation of local moment balance \( dM = Tdu \), where \( M(x) \) is the bending moment. Dividing both sides by the length of the section, \( dx \), one has the third-order equation of shearing force equilibrium [7]

\[
\kappa \frac{d^3u}{dx^3} = T(x) \frac{du}{dx}.
\]

(2)

again valid for small transverse deflections \( u(x) \) confined to a plane. Regions of \( T > 0 \) correspond to tension, while regions of \( T < 0 \) correspond to compression. The textbook application of Equation (2) (treated in Ref. [7]) is to a vertical column of height \( h \) that buckles under its own weight: \( T(x) = -\sigma(h-x) \), where \( \sigma \) is the weight per unit length. By a change of variable \( w \equiv du/dx \), Equation (2) takes the form of the 1d Schrödinger equation

\[
\kappa \frac{d^2w}{dx^2} = T(x)w.
\]

(3)

This is similar in appearance to the second-order equation of moment equilibrium obtained by integrating Equation (2) for the special case of constant \( T \). That result, \( \kappa u'' = Tu \), is commonly known as the Euler buckling equation. It should be clear, however, that Equation (3) is more general than the Euler buckling equation, and it also has a different physical meaning. Boundary conditions for Equations (2) and (3) typically involve hinged or clamped rod ends, and solutions \( u(x) \) and \( w(x) \) to such...
boundary value problems describe unstable equilibrium configurations of the rod, i.e., elastic instabilities.

Letting $\mathbf{r} = r_x \hat{x} + r_y \hat{y}$ be the displacement vector that locates one end of the rod with respect to the other, we define a “projected length” of the rod as $L \equiv |r_x|$. In an unstable equilibrium configuration, the rod’s contour length $L_C$ exceeds $L$ by an amount

$$L_C - L = \int_0^L dx (\sqrt{1 + w^2} - 1) \approx \frac{1}{2} \int_0^L dx w^2.$$ \hspace{1cm} (4)

Mechanistically, the elastic instability exchanges some of the axial compressive and/or tensile stress for bending stress, thus $L_C$ is also comparable to the relaxed length of the rod, and we may define a critical strain for the instability as $\gamma_c \equiv (L_C - L)/L$. The validity conditions for both Equations 2 and 3 as well as the small $w$ expansion in Equation 4 can now be expressed as $\gamma_c \ll 1$. In the limit $\gamma_c L \to 0$, which allows for the possibility that $L \to \infty$, Equation 4 can be written as

$$\int_0^L dx \left( \frac{w}{\sqrt{2 \gamma_c L}} \right)^2 = 1.$$ \hspace{1cm} (5)

So in this limit, which is equivalent to the WLC limit, not only does the slope $w(x)$ satisfy a Schrödinger-like equation, it satisfies an inextensibility constraint that is reminiscent of normalization.

Introducing a rescaled slope $W(x) \equiv w(x)e^{-i\phi}/\sqrt{2 \gamma_c L}$ that is dimensionally consistent with a 1d quantum mechanical wavefunction, where $\phi$ is an arbitrary constant phase angle, Equations 3 and 5 become

$$\frac{d^2 W}{dx^2} - \frac{\kappa}{\lambda} T(x) W = 0,$$

$$\int dx |W|^2 = 1.$$ \hspace{1cm} (6, 7)

The integration is over the projected length of the WLC. Evidently the problem of generalized elastic instabilities in WLCs maps to 1d, nonrelativistic, time-independent quantum mechanics according to

$$\frac{w(x)}{\sqrt{2 \gamma_c L}} \rightarrow e^{i\phi} \psi(x),$$ \hspace{1cm} (8)

$$-\frac{T(x)}{\kappa} \rightarrow \frac{p^2(x)}{\hbar^2},$$ \hspace{1cm} (9)

where $\psi(x)$ is a normalized wavefunction in which any and all relative phase differences are restricted to integer multiples of $\pi$. The global phase factor $e^{i\phi}$ makes the (possibly complex) wavefunction real-valued but has no physical significance, and $p(x) = \sqrt{2m[E - V(x)]}$. Regions of compression of the WLC map to classical regions: $E - V(x) > 0$, while regions of tension map to nonclassical regions: $E - V(x) < 0$. A neutral “surface” of the WLC maps to a classical turning point in the quantum problem. A boundary condition in which the WLC is clamped parallel to $\hat{x}$ (but the clamp can slide transversely) maps to a boundary condition in which the wave function vanishes.

Further aspects of the mapping are obtained from the deformation energy of the unstable equilibrium configuration. Let $H_{\text{bend}}$ and $H_{\text{stretch}}$ denote the first and second terms on the right hand side of Equation 1. Inserting Equation 3 and integrating by parts, we find

$$H_{\text{bend}} \rightarrow \frac{\hbar^2}{\kappa} \frac{\langle |\psi|^2 \rangle}{\langle \psi | p^2 | \psi \rangle}.$$ \hspace{1cm} (10)

The choice $\kappa \gamma_c L = \hbar^2/2m$ maps the bending energy directly to the expectation value of the kinetic energy. Next we observe that the axial stress is $T(x)(1 - w^2(x))/A$, where the numerator is the component of $T(x)\hat{x}$ parallel to the WLC’s axis in the small angle approximation. By Hooke’s Law the axial strain is $T(x)(1 - w^2(x))/\mu$. Inserting this and Equation 5 into Equation 1 we find to leading order

$$\frac{2 \mu H_{\text{stretch}}}{\kappa^2} \rightarrow \frac{1}{\hbar^2} \int dx p^4(x),$$ \hspace{1cm} (11)

with a next order correction $\sim \langle |\psi|^4(x) | \psi \rangle$.

Below we examine four sample applications of the mapping that span a wide range of qualitative behaviors. The first two involve only contact forces, while the latter two involve body forces.

**Particle in a box** — The elastic instability problem analogous to a particle in a 1d infinite square well of width $L$ is

$$w'' + q^2 w = 0, \quad w(0) = w(L) = 0,$$ \hspace{1cm} (12)

where $q^2 = -T/\kappa > 0$. Physically, this represents an axially compressed WLC whose ends are clamped but the clamps are free to slide transversely. The eigenvalues and eigenslopes are given by $\lambda_n = n^2 \pi^2 \kappa/L^2$ and $w_n(x) = 2\sqrt{\gamma_c} \sin(n \pi x/L)$, respectively, and the first few of these are shown in Figure 1. One can easily verify that the eigenslopes satisfy the inextensibility constraint (Equation 6) and the mapping to the normalized $\psi_n$ (via Equation 8). The eigenvalues of the two problems are related by $2m E_n/\hbar^2 = -\lambda_n/\kappa$, consistent with Equation 9. The general solution to Equation 12 is a linear combination of eigenvalues, and the WLC’s shape $w(x)$ is found by integrating that combination.

Let us examine a superposition of eigenslopes involving a relative phase difference: $w(x) \sim \sin(n_1 \pi x/L) \pm \sin(n_2 \pi x/L)$. The bending energy density (integrand of the first term in Equation 1) contains a phase-dependent term $\sim \pm \cos(n_1 \pi x/L) \cos(n_2 \pi x/L)$ that integrates to zero when $n_1 \neq n_2$, but is nevertheless related to an observable. Imagine constructing a thin rod (WLC) out of a photo-elastic material such as polycarbonate, and then shining polarized light on the buckled rod. The resulting
birefringence pattern would be different for the (+) superposition than for the (−) superposition, because these correspond to different states of bending stress \( \sim \frac{dT}{dx} \). So even though relative phase differences are here restricted to be integer multiples of \( \pi \) since the entity analogous to the wavefunction is real-valued, such phase differences can lead to observable consequences as they also do in quantum mechanics.

What are the consequences of choosing \( \kappa \gamma_c L = \hbar^2/2m \), which maps the bending energy directly to the kinetic energy, as mentioned above? One consequence would be that the buckling force is \( -T_n = E_n/\gamma_c L \), much larger than the force required to adiabatically change the width of the well \( -dE_n/dL = 2E_n/L \). Is that problematic? No, in fact it is entirely reasonable behavior given that adiabatically changing the width of the well corresponds to changing the projected length of the already-buckled WLC. (Engineers consider buckling to be a mode of failure precisely because a generic rod can support a much greater axial load prior to buckling than after it has buckled, and a WLC is no exception to this rule.) Another consequence is thermodynamic in nature. A fundamental property of a WLC is its persistence length \( L_p = \frac{2\kappa}{\gamma_c} \) (in 2d), defined as the decay length of the tangent-tangent correlation function \( \langle \hat{t}(s) \cdot \hat{t}(s') \rangle = \exp(-|s-s'|/L_p) \). Here \( \tau \) is the Boltzmann constant times temperature, and \( \hat{t}(s) \) is the unit vector tangent to the WLC at distance \( s \) measured along its contour length. Since the mapping is valid only for small transverse deflections of the WLC, we must be confined to the “stiff” regime \( L \lesssim L_p \), i.e., the low temperature regime of the WLC [9]. Under this restriction, we would have \( \sqrt{2\pi \gamma_c L_p} = \lambda_{th} \), where \( \lambda_{th} \) is the thermal average wavelength of the particle in a box, i.e., a 1d ideal gas of density \( L^{-1} \). Inserting the condition \( L \lesssim L_p \) into the last equation indicates the ideal gas would be in the density regime \( L^{-1} \lesssim \sqrt{2\pi \gamma_c L_p} \), where \( \lambda_{th}^{-1} \) is known as the quantum concentration. However, since \( \gamma_c \to 0 \), this is not actually a restrictive condition; the cold WLC picture would hold regardless of whether the ideal gas is in the quantum or classical regime (density above or below \( \lambda_{th}^{-1} \), respectively).

**Particle in a delta-function well** — The time-independent Schrödinger equation

\[
\frac{-\hbar^2}{2m} \frac{d^2 \psi}{dx^2} - g\delta(x)\psi = E\psi, \tag{13}
\]

can be recast as separate boundary value problems for each half-space. For the positive half-space,

\[
\psi'' - k^2 \psi = 0, \quad \psi(\infty) = 0, \quad \psi'(0) = -\frac{1}{R} \psi(0), \tag{14}
\]

where \( k^2 = 2m|E|/\hbar^2 \), \( R = \hbar^2/mg \), and the second boundary condition comes from integrating Equation (13) across an infinitesimal region centered on the origin. The sole bound state solution is \( \psi(x) = \sqrt{1/R} e^{-x/R} \), and the energy of this state is \( E = -mg^2/2\hbar^2 \).

The analogous elastic instability problem has been described by Misseroni, et al. [11]: clamp one end of a rod and constrain the clamp to slide along a circular path having radius \( R \), then pull on the other end (see Figure 1). Here the rod is an infinitely long WLC, so the boundary value problem is

\[
w'' - q^2 w = 0, \quad w(\infty) = 0, \quad w'(0) = -\frac{1}{R} w(0), \tag{15}
\]

where \( q^2 = T/\kappa > 0 \). The WLC will remain straight until the tension reaches a critical value \( T = \kappa/R^2 \), at which point it will deflect and acquire slope \( w(x) = \sqrt{2\gamma_c L/R} e^{-x/R} \). (Recall \( \gamma_c L \to 0 \) is implicit here.) Just as there is only one bound state for the delta-function well, there is only one “buckling” mode for the tensioned rod. The binding energy and buckling force are related by \( E = -\hbar^2 T/2m\kappa \), again consistent with Equation (9).

**Particle in a triangular well** — While the previous two applications involved only contact forces (applied to the ends of the WLC and transmitted throughout its length as required by force balance), this application involves both contact forces and a body force. First we consider the quantum problem of a particle in a potential well \( V(x) = \eta x \) for \( x > 0 \) and \( V(x) = \infty \) for \( x < 0 \), where \( \eta \) is a constant force. Physically, this could describe an electron near a doped heterojunction [12]. Schrödinger’s equation is given by

\[
\psi'' - \frac{2m\eta}{\hbar^2} \left( x - \frac{E}{\eta} \right) \psi = 0, \quad \psi(0) = \psi(\infty) = 0. \tag{16}
\]
The stationary states (plotted in Figure 2) are
\[ \psi_n(x) = \frac{\sqrt{\eta/\epsilon_0}}{\text{Ai}'(a_n)} \text{Ai}\left( \frac{\eta x - E_n}{\epsilon_0} \right), \]
where Ai(z) and Ai’(z) denote the Airy function and its derivative, \( E_n = |a_n|\epsilon_0 \),
\[ \epsilon_0 = \left( \frac{\eta \hbar^2}{2m} \right)^{1/3}, \]
and \( a_n < 0 \) is the \( n \)th zero of the Airy function. The normalization of Equation 17 can be verified using an integral identity given in Ref. 13. The analogous elastic instability problem is a variation on the “self-buckling” scenario described earlier. Suppose a massive WLC is oriented parallel to a uniform gravitational field. It is both supported from its bottom (at \( x = 0 \)) and suspended from its top (at \( x = L \)), such that it has a neutral “surface” at some height \( x_0 \) between 0 and \( L \). The axial force is \( T(x) = -\sigma(x_0 - x) \). Both ends of the WLC are clamped, but the clamps are free to slide transversely as in the previous two applications. For \( L \to \infty \), the boundary value problem describing shearing force equilibrium is
\[ w'' - \frac{\sigma}{\kappa}(x - x_0)w = 0, \quad w(0) = w(\infty) = 0. \]
This is identical to Equation 16 when \( \sigma/\kappa = 2m\eta/\hbar^2 \), and \( x_0 = E/\eta \). The classical turning points \( E_n/\eta \) in the quantum problem become the neutral surfaces \( (x_0)_n \) in the elastic problem (see Figure 2).

Many interacting particles... What is the elastic instability counterpart of a quantum many-body problem? As a very basic starting point, we show how a Hartree-like term \[ 13 \] could arise for a “bundle” of interacting WLCs. First we revisit Equation 4 and notice that, physically, \( w^2(x)/2 \) is the “excess length density,” i.e., the fraction of the WLC’s total excess length \( L_C - L \) found between \( x \) and \( x + dx \). Suppose the WLC had a charge uniformly spread over its contour length; the charge per unit projected length would be \( \sim C + w^2(x) \), where \( C \) is a constant. Now consider a bundle of charged WLCs that are all in unstable equilibrium configurations (but not necessarily the same configuration). If the charged WLCs have 2d electrostatic interactions with one another, then the magnitude of the body force on the \( i \)th WLC from all the others is
\[ F_i(x) \sim \sum_{j \neq i} \int dx' \frac{\text{Ai}\left( \frac{\eta x - E_n}{\epsilon_0} \right) C + w_j^2(x')}{\sqrt{(x - x')^2 + (u_i(x) - u_j(x'))^2}}. \]
(20)
(Here the subscripts label WLCs, not modes of instability.) Since the \( u \)’s and \( w \)’s are small quantities, the transverse component of the body force is small, and Equation 20 is well approximated by
\[ T_i(x) \sim \sum_{j \neq i} \int dx' \frac{\text{Ai}\left( \frac{\eta x - E_n}{\epsilon_0} \right) C + w_j^2(x')}{|x - x'|}. \]
(21)
The divergent part of this integral can presumably be discarded, and what remains is a Hartree-like contribution to the total force \( T(x) \) exerted on the \( i \)th WLC.

We have shown by a formal mapping, and by several applications of that mapping, that many of the features of non-relativistic, time-independent quantum mechanics are also contained within a certain class of elastic instability problems. In these problems, the product of a WLC’s bending stiffness and critical buckling strain plays the role of \( \hbar^2/mL \), and the derivative of the buckled WLC’s shape plays the role of the normalized wavefunction. A statement of shearing force balance in the elastic problem is analogous to the statement of energy conservation that is embodied by the Schrödinger equation. As mentioned in the first paragraph, other quantum-buckling analogies can and have been made using second and fourth-order elastic equations. However, these other analogies do not appear to have the combination of generality (in the sense of arbitrary \( V(x) \)) and depth (in the sense that the dependent variable simultaneously satisfies a normalization-like constraint) that is inherent to the third-order equation of shearing force balance.

In principle, more complicated applications exist than the simple ones we’ve considered here, although whether these correspond to physically realistic scenarios on both sides of the analogy is left as an open question. For instance, what would be the quantum analog of a substrate
term in the elastic equations? What would be the elastic analog of an exchange term in the many-body problem? Is it possible that an intractable problem on one side can be mapped to a less difficult or more intuitive problem on the other side? Also, one might ask whether the formal mapping above can be generalized to higher dimensions. The consideration of time-dependence in the elastic instability problem, and whether that resembles time-dependence in quantum mechanics, is another possible line of inquiry. This work establishes a theoretical foundation, and provides several intuition-building examples, from which further such questions can be addressed.

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