Dynamics of Kirchhoff rods and rings from a minimal coupling quantum isomorphism

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A minimally coupled nonrelativistic quantum particle in 1d is shown to be isomorphic to a much heavier, vibrating, very thin Euler-Bernoulli rod in 3d, whose ratio of bending modulus to linear density is $(\hbar/2m)^2$. Axial body forces and terminal twisting couples acting on the rod play the role of scalar and vector potentials, respectively, and within the semiclassical approximation, rod inextensibility plays the role of normalization. Orbital angular momentum quantized in units of $\hbar/2$ emerges when the force and couple-free inextensible rod is formed into a ring, and the ring vibrates in a toroidal helix mode. The isomorphism suggests something akin to wavefunction collapse occurs in dynamical buckling, and further suggests how to construct a new kind of classical analog of a 1d Bloch electron.

Introduction.— Mathematical analogies between quantum mechanical systems and vibrating elastic systems have been made since the earliest days of quantum mechanics, when in 1926, Schrödinger observed that the "square" of what we now think of as the time-dependent Schrödinger equation resembles the equation of motion of a vibrating plate [1, 2]. Looking at this in reverse, the Euler-Bernoulli operator for a freely vibrating plate can be factored into two Schrödinger-like operators: $\partial_t^2 + \Delta^2 = (i\partial_t + \Delta)(-i\partial_t + \Delta)$, a property useful in certain solution schemes [3, 4], while it has similarly been shown that the Föppl-von Kármán operator describing large deflections of the plate can be factored into two nonlinear Schrödinger-like operators [5]. However, such analogies are fundamentally limited by the fact that the real, scalar transverse plate deflection or some derivative thereof stands in for a complex wavefunction. A closer continuum elastic analogy can be made to *one-dimensional* quantum mechanics, and this involves a rod or elastica that deflects in two transverse dimensions. Here the components of the deflection vector (or even more powerfully, as we will see, the components of the transverse projection of the tangent vector) can play the roles of $\mathrm{Re}[\Psi]$ and $\mathrm{Im}[\Psi]$. While aspects of the 1d quantum - 3d rod analogy have appeared in the literature before, the focus has been on time-independent phenomena [6–11], specific forms of interaction relevant to semiflexible polymer systems [6–8], and nonlinear effects such as bend-twist coupling [9, 10], rather than on pushing the linear time-dependent analogy to the point of becoming an isomorphism, as we do here.

The value of such an isomorphism is, of course, in the potential to learn something about elastic systems from quantum systems, and vice versa, just as analogies between the band structure of electronic systems and vibrations of isostatic frames [12], metamaterials [13], jammed packings [14], and continuous plates with patterened resonators [15] have recently been used to predict the existence of topologically protected edge modes in the latter four. As a more historic example, de Gennes showed that quantum fluctuations of a 1d Fermi gas can be mapped to thermal fluctuations of 2d polymeric systems (albeit flexible, not semiflexible polymers), where a "no-crossing" condition for polymer chains plays the role of Fermi statistics [16].

While both the quantum and classical elastic systems considered here are comparatively simple, we nevertheless gain some surprising insights in both directions. We find, for example, that subject to a spatially periodic body force such as might be generated by interactions within the rod, a vibrating rod can constitute a classical analog of a 1d Bloch electron (distinct from a phononic crystal in that the vibrations are flexural). Also, when an elastic *ring* — whose properties of inextensibility and bending modulus to linear density ratio are fixed by the isomorphism — vibrates in a toroidal helix mode, its orbital angular momentum can take on the character of quantum spin. The key to all this turns out to be the higher order and therefore virtually unused "squared" Schrödinger equation.

Formalism.— Consider a quantum particle with wavefunction $\Psi(\mathbf{r},t) = \Psi_1(\mathbf{r},t) + i\Psi_2(\mathbf{r},t)$, Ψ_1 and Ψ_2 being real, that satisfies the time-dependent Schrödinger equation $i\hbar\partial_t\Psi = \hat{H}\Psi$. This problem is isomorphic to

$$\begin{pmatrix} 0 & -\hbar\partial_t \\ \hbar\partial_t & 0 \end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} = \begin{pmatrix} \mathrm{Re}[\hat{H}] & -\mathrm{Im}[\hat{H}] \\ \mathrm{Im}[\hat{H}] & \mathrm{Re}[\hat{H}]\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}, \quad (1)$$

written more concisely as

$$R\Big(\frac{\pi}{2}\Big)\hbar\partial_t\vec{\Psi} = \tilde{H}\vec{\Psi}, \quad (2)$$

where $R(\pi/2)$ is a $\pi/2$ rotation matrix, $\tilde{H}$ denotes the matrix of operators on the right hand side of Eq. (1), and $\vec{\Psi}(\mathbf{r},t) = (\Psi_1(\mathbf{r},t), \Psi_2(\mathbf{r},t))$ is a vector function in the now real, but 2×higher dimensional Hilbert space: $\mathbb{R}^2(\mathbb{R}^d)$ versus $\mathbb{C}(\mathbb{R}^d)$. (To avoid ambiguity, we use arrow notation and boldface for vectors in $\mathbb{R}^2$ and $\mathbb{R}^d$, respectively.)

The Hamiltonian of interest in this work is the minimal coupling Hamiltonian

$$\hat{H} = \frac{1}{2m}\big(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}(\mathbf{r},t)\big)^2 + V(\mathbf{r},t), \quad (3)$$

corresponding to

$$\tilde{H} = -\frac{1}{2m}\begin{pmatrix} \hbar\boldsymbol{\nabla} & q\mathbf{A} \\ -q\mathbf{A} & \hbar\boldsymbol{\nabla} \end{pmatrix}^2 + \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix}. \tag{4}$$

In this limited context, we refer to Eq. (2) as the real time-dependent Schrödinger equation (rTDSE).

Assuming time-independent $\tilde{H}$, Eq. (2) has general "normalized" solution

$$\vec{\Psi}(\mathbf{r}, t) = \sum_n R(-\omega_n t) c_n \vec{\psi}_n(\mathbf{r}), \tag{5}$$

where $\hbar^{-1}\tilde{H}\vec{\psi}_n = \omega_n\vec{\psi}_n$, $\delta_{nm} = \int d\mathbf{r}\,\vec{\psi}_n \cdot \vec{\psi}_m$, and $1 = \sum_n c_n^2$. Note the identity $R(\alpha) = \exp[\alpha R(\pi/2)]$, Euler's formula for 2d rotations. The $\vec{\psi}_n$ are, in general, nonplanar due to $\mathbf{A}$, they rotate at angular frequencies ω_n, and they correspond to stationary states. That is, if $\psi_n = \psi_{n,1} + i\psi_{n,2}$ is an eigenstate of $\hat{H}$ with eigenvalue E_n, then $\vec{\psi}_n = (\psi_{n,1}, \psi_{n,2})$ is an eigenstate of $\tilde{H}$ with the same eigenvalue. Equation (5) is also a solution of the higher order equation

$$-\hbar^2\partial_t^2\vec{\Psi} = \tilde{H}^2\vec{\Psi}, \tag{6}$$

obtained by operating on both sides of Eq. (2) with $R(\pi/2)\hbar\partial_t$. As its complex counterpart is sometimes called the "squared" Schrödinger equation, we refer to Eq. (6) as the real squared Schrödinger equation (rSSE).

What is gained by the transformation to the rSSE (which also holds for adiabatically slow changes in the sense $[\partial_t, \tilde{H}] \approx 0$) is a new, indeed classical, interpretation of $\vec{\Psi}$. When $d = 1$, and not-very-restrictive conditions are imposed on V and $\mathbf{A}$, $\vec{\Psi}$ describes a thin elastic rod that dynamically and helically buckles in $\mathbb{R}^3 = \mathbb{R}^2 \otimes \mathbb{R}^d$. Furthermore, the normalization condition becomes an inextensibility constraint within the rod context, and within an approximation equivalent to the semiclassical approximation. Armed with this physical understanding, we specialize to those solutions of the rSSE that are also solutions of the lower order rTDSE, and use elementary quantum mechanics as a guide to elucidate the properties of this elastic rod.

Dynamically and helically buckled rod.— When $d = 1$, $V = V(x)$, and A_x is constant with respect to x, the rSSE can be written as the following set of coupled equations:

$$-\rho\ddot{\Psi}_1 = B\Psi_1'''' + M\Psi_2''' + (P\Psi_1')' + K\Psi_1 + C\Psi_2' + (C'/2)\Psi_2, \tag{7a}$$
$$-\rho\ddot{\Psi}_2 = B\Psi_2'''' - M\Psi_1''' + (P\Psi_2')' + K\Psi_2 - C\Psi_1' - (C'/2)\Psi_1. \tag{7b}$$

Dots and primes denote partial derivatives with respect to t and x, respectively, while $B/\rho = (\hbar/2m)^2$, $M/\rho = \hbar q A_x/m^2$, $P/\rho = -V/m - 3M^2/8\rho B$, $K = (P + M^2/4B)^2/4B + P''/2$, and $C = P(M/2B) + B(M/2B)^3$.

Apart from terms involving C that we momentarily ignore, Eqs. (7) are the 3d equations of motion of an Euler-Bernoulli beam with circular cross section, also known as a Kirchhoff rod. Table I suggests its scale. The rod undergoes transverse deflection from the x-axis proportional to $\vec{\Psi}$, has mass per unit length ρ and bending modulus B, and sustains both an axial moment (torque) M and an axial body force $P(x)$. ($P > 0$ where the rod is in compression and $P < 0$ where it is in tension.) Notice that P accounts for twist-induced tension, suggesting the internal structure of the rod is a bundle of inextensible fibers [18]. This picture is consistent with a single-valued bending modulus for the composite rod structure provided there is no cross-linking [17]. The rod also experiences a "substrate" force, e.g., from being embedded in an elastic gel, with force constant per unit length $K(x)$. The case of Eqs. (7) with $M = K = C = 0$ and $P > 0$ is known as the dynamical buckling equation [19–21], yet the extra features described above are well-studied extensions of linear buckling [22–24], if not typically together and in a dynamical context. Counterintuitively, even when a rod is everywhere in tension it can buckle given suitable boundary conditions [25]. The case of Eqs. (7) with $P = K = C = 0$ describes flexural vibration of a rod with pre-twist [26].

TABLE I. Rods described by the rSSE are comparable in scale to semiflexible polymers, typically modeled as wormlike chains [17]. Examples of these are indicated with asterisks. Entries are in units of $\mathrm{m}^4/\mathrm{s}^2$.

	$(\hbar/2m)^2$	B/ρ [a]
proton	9.8×10^{-16}	
electron	3.3×10^{-9}	
DNA*		$\sim 10^{-13}$
microtubule*		$\sim 10^{-10}$
20 μm diameter glass fiber		$\sim 10^{-3}$
16 ga. steel wire		~ 1

[a] $B = \frac{\pi}{4}ER^4 = k_BT\ell_P$, where E is the rod's Young's modulus, R is its radius, and ℓ_P is its persistence length in 3d. Thus B/ρ scales as R^2 times the specific Young's modulus.

As $x \to 0$, the second and fifth terms on the right hand sides of Eqs. (7) can be combined into $\pm(\mathcal{M}\Psi_{2,1}')''$ where $\mathcal{M}(x) = M + C(x)x^2/2$. So at least for part of

the rod, the physical effect of C is to generate a variable axial moment [24]. However, we will avoid further complications introduced by the C and C' terms by assuming M, P, and P' are everywhere small compared to B/R, B/R^2 and B/R^3, respectively, where R is the rod's radius. When the rod's aspect ratio is that of a semiflexible polymer, these are not very restrictive conditions. And since $M = B\tau/(1+\nu)$, where τ is the torsion (rate of twist) and ν is Poisson's ratio, the first condition can be restated as small torsional strain $R\tau$. Thus only terms up to linear order in MR/B, PR^2/B, and $P'R^3/B$ and are retained in the nondimensionalized equations of motion (lengths measured in units of R, time in units of $R^2\sqrt{\rho/B}$), simplifying the latter three coefficients in Eqs. (7) to $P/\rho = -V/m$, $K/\rho = -V''/2m$, and $C = 0$. Within this approximation and in rod language,

$$\frac{\tilde{H}}{\hbar} = -\sqrt{\frac{B}{\rho}}\begin{pmatrix} \partial_x & M/4B \\ -M/4B & \partial_x \end{pmatrix}^2 - \frac{P(x)}{2\sqrt{\rho B}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (8)$$

If $P(x)$ varies slowly on the scale of the rod length, Eqs. (7) further reduce to

$$-\rho\ddot{\Psi}_1 = B\Psi_1'''' + M\Psi_2''' + P\Psi_1'', \quad (9a)$$
$$-\rho\ddot{\Psi}_2 = B\Psi_2'''' - M\Psi_1''' + P\Psi_2''. \quad (9b)$$

The essentially constant coefficients arising from this "semiclassical" approximation mean that $\vec{\Psi}$ can now be interpreted as any scaled derivative of the transverse deflection $\vec{u}(x,t) = u_1(x,t)\hat{y} + u_2(x,t)\hat{z}$. A particularly compelling choice is $\vec{\Psi} = \vec{u}'/\sqrt{2\gamma L}$, as this gives rise to a geometrical constraint $1 = \int dx\vec{\Psi}\cdot\vec{\Psi}$ if the rod is inextensible, i.e., if its contour length is conserved. Here L is the projected (onto the x-axis) length of the rod, and γ is its relative compression (not to be confused with axial strain, and not implying that $P > 0$); the inextensibility constraint written above is the leading order term in an expansion and so is valid only when $\vec{u}'\cdot\vec{u}' \ll 1$ everywhere, meaning $\gamma \ll 1$. Inextensibility is a good assumption for semiflexible polymers — it being an ingredient of the wormlike chain model [17] — and is consistent with the internal structure of the rod inferred earlier, even though that structure is not accounted for at linear order in MR/B. Equations (9) have another interesting feature in that static helically buckled configurations of the rod (zero modes of $\tilde{H}^2\vec{\psi} = E^2\vec{\psi}$) map onto the dynamics of a symmetric top that remains nearly upright and has its bottom point fixed [22].

Setting aside the broader analogy that can be made without the semiclassical approximation in favor of the deeper one that can be made with it, we proceed for now with Eqs. (9) and assign $\vec{\Psi} = \vec{u}'/\sqrt{2\gamma L}$ except where otherwise indicated. Notice that the linear equations of motion do not discriminate between ρ as mass per unit length in the x-direction and ρ as mass per unit contour length (the local conversion factor being $1+\gamma L\Psi^2$), and therefore, we are free to choose the latter definition, which is the more realistic for an inextensible rod. A consequence is that purely transverse vibration of the inextensible rod is associated with a longitudinally propagating momentum. This can be seen by combining the continuity equation $\partial_t[\rho(1+\gamma L\Psi^2)] + \partial_x g = 0$ with Eqs. (2) and (4) to obtain the momentum density

$$g(x,t) = -2\gamma L\sqrt{\rho B}\left[\vec{\Psi}\cdot R\Big(\frac{\pi}{2}\Big)\vec{\Psi}' + \frac{M}{4B}\Psi^2\right]. \quad (10)$$

Comparing to the quantum mechanical momentum density, i.e., m times the probability current $-(\hbar/m)\{\mathrm{Re}[\Psi^* i\Psi'] + (qA_x/\hbar)|\Psi|^2\}$, leads to the identification $\hbar = 2\gamma L\sqrt{\rho B}$ in terms of rod parameters. Putting this in the relationship $B/\rho = (\hbar/2m)^2$ further identifies $m = \rho\gamma L$. This result makes intuitive sense: the rod has mass ρL (to leading order), and so the pulse mass set in motion by a relative compression γ is $\rho\gamma L$ (to leading order). In other words, the isomorphism connects a massive quantum particle with a much more massive (by a factor of γ^{-1}) elastic rod. When $M = P = 0$, Eq. (10) reduces to the standard geometrical result for inextensible strings, ropes, and rods: $g(x,t) = -\rho\partial_x\vec{u}\cdot\partial_t\vec{u}$. To see this, use $\vec{u}$ as the dependent variable in Eq. (2), which is a valid procedure within the semiclassical approximation as discussed above.

Guided by Eq. (10), we can now write down the free energy functional from which Eqs. (9) can be obtained:

$$F = \frac{1}{2}\int dx\Big[B(\vec{u}'')^2 + M\vec{u}'\cdot R\Big(\frac{\pi}{2}\Big)\vec{u}'' - P(\vec{u}')^2\Big]. \quad (11)$$

The last two terms are isomorphic to $\int dx A_\mu j^\mu$ of classical electrodynamics (to linear order in MR/B). Here, making use of our previous results, $qA_\mu = -\gamma L(P, \sqrt{\frac{\rho}{4B}}M, 0, 0)$ and $j^\mu/q \leftrightarrow (\Psi^2, g/\rho\gamma L, 0, 0)$.

Ring vibrating in a toroidal helix mode.— For a sample application of the momentum density, we consider the n^{th} helical eigenstate and corresponding eigenfrequency of Eq. (8):

$$\vec{\psi}_n(x) = \frac{1}{\sqrt{L}}R(k_n x)\hat{y}, \quad (12a)$$
$$\omega_n = \sqrt{\frac{B}{\rho}}(k_n - q)^2 - \frac{P}{2\sqrt{\rho B}}, \quad (12b)$$

where $k_n = 2\pi n/L$, $q = M/4B = \phi/4L(1+\nu)$, and ϕ is the total twist over length L. This describes a mode of vibration of a rod with periodic boundary conditions; alternatively, it describes a continuous ring of radius $L/2\pi$ if we neglect effects of the undeformed ring's curvature (compare the model in Ref. [19]). Such neglect is justified when $R^2 \ll (L/2\pi)^2$, and in any case, accounting for the curvature would introduce corrections to P and K that couple only to the in-plane component of $\vec{\Psi}$ [20, 23] — interesting, but incompatible with the isomorphism here.

The ring deflection corresponding to Eqs. (12) is, up to a rigid translation of the guiding center,

$$\vec{u}_n(x,t) = -\frac{\sqrt{2\gamma}}{k_n} R(k_n x - \omega_n t)\hat{z}. \tag{13}$$

Letting the plane of the ring be perpendicular to the z-axis, Eq. (10) gives orbital angular momentum $L_z = gL^2/2\pi = \hbar(n - \phi/8\pi(1+\nu))$. If ϕ is zero or an integer multiple of $8\pi(1+\nu)$, L_z is quantized in units of $\hbar$. Of course, when we say "units of $\hbar$" we are assuming the factor of length change γL in $\hbar$ is independent of n, which is not intuitive for elastic rings. And yet the isomorphism is telling us that γL for this particular elastic ring is indeed independent of n.

Intriguingly, a variety of different approaches show that the standard result for g quoted above is missing a factor of 1/2 [27]. One simple way to see the discrepancy is to first write the linear momentum as the pulse mass times the pulse velocity: $\int dx g = \rho\gamma L(\omega_n/k_n) = \frac{1}{2}\rho(\omega_n/k_n)\int dx \vec{u}'\cdot\vec{u}'$. Next observe that Eq. (13) satisfies $\vec{u}' = -(k_n/\omega_n)\partial_t\vec{u}$, and substitute this for one factor of $\vec{u}'$ in the integrand. For another particularly relevant perspective, see Juenker's kinetic energy analysis of traveling helical waves in inextensible strings [28]. Their Eqs. (8), (15), and (19), when expressed in our notation and setting $M = P = 0$, read $gL = 2\pi n\gamma\sqrt{\rho B}$. All of this points to L_z quantization in units of $\hbar/2$ (for $M = P = 0$), and one cannot help but compare the situation here (i.e., certain methods giving roughly twice as many solutions as others) with the situation for spin, which, as every student of quantum mechanics learns, yields to an operator method but defies an apparently rigorous series-solution method.

Letting Eqs. (12) describe the periodic straight rod rather than the ring gives rise to yet another kind of orbital angular momentum, also discussed by Juenker: $L_x = \int dx \rho u_n^2 \omega_n = \hbar$ (for $M = P = 0$). Because the rod is now infinitely long (in a sense), and is in a helical mode that carries both L_x and $p_x = gL$, it is reminiscent of an OAM beam [29].

A final feature of note regarding the ring is that its quantum counterpart is a charged particle confined to a loop threaded by a magnetic flux — the starting point of topological quantum field theory [30]. Just as in that setting, a gauge transformation $\vec{\psi}_n(x) = R(-qx)\vec{\eta}_n(x)$ here removes the twist at the expense of a discontinuity in the boundary conditions. The discontinuity vanishes when qL is an integer multiple of 2π, indicating an extension of the Byers-Yang theorem: all physical properties of the ring are periodic in twist ϕ, with period $8\pi(1+\nu)$ between 4 ($\nu = 0$) and 6 ($\nu = 1/2$) complete twists, assuming the small torsional strain condition remains satisfied.

Mode selection and mode coarsening.— Conventionally in dynamical buckling (where $M = 0$ and P is a positive constant), one assumes that a perturbation with wave number k grows at rate $\sigma(k)$. This leads to a prediction that the fastest-growing, hence, most probable mode is the one with $k = \sqrt{P/2B}$, a result that is in good agreement with experiments on rings confined to buckle in plane [19]. The natural question to ask in the present context, however, is not which mode is selected out of an unbuckled state, but which mode is selected out of a superposition state, i.e., what is the analog of wavefunction collapse? In light of the isomorphism, the natural candidate for the probability that, e.g., ω_n is the outcome of a measurement of ω, would appear to be c_n^2. But it bears repeating that whereas in quantum mechanics $1 = \sum_n |c_n|^2$ is (an initial condition on) a postulate, for a Kirchhoff rod $1 = \sum_n c_n^2$ is a consequence of the physical condition of inextensibility.

The isomorphism also gives a possible new perspective on the mode coarsening behavior recently observed in experiments on dynamically buckled rods [21]. The observed scaling behavior $k \sim t^{-1/1.9}$ is close to $k \sim t^{-1/2}$, what one would expect from first order time-dependent perturbation theory when the potential (buckling force) is a step function at $t = 0$. This scaling relation follows from the fact that transitions in such a scenario have appreciable probability only if the change in mode frequency $\Delta\omega \sim (\Delta k)^2 \sim t^{-1}$ [31]. A big caveat, however, is that the derivation of the rSSE from the rTDSE assumes adiabatically slow time dependence, and this assumption is almost certainly violated for impact forces such as those used in Ref. [21]. What happens to the isomorphism under more general time-dependent forces, including impact forces and longitudinal sound waves, is certainly an interesting direction for future work.

Classical analog of a Bloch electron.— Let us return to Eq. (8) and forgo making the semiclassical approximation so that $\vec{\Psi} \sim$ rod deflection and $P(x)$ is an arbitrary smooth function (as $R/L \to 0$). A convenient property of the isomorphism is that if P is a sinusoidal function, so is K (implicit in Eq. (8)). This suggests *engineering* out-of-phase sinusoidal variations in the axial body force and in the substrate stiffness. One way to achieve the former could be by manipulating intrachain interactions in a stiff polyelectrolyte — already implicated in buckling [8] — by creating an alternating pattern of charged and neutral monomer blocks [32]. If such a polymer were made to vibrate in a non-dissipative environment of similar polymers, all parallel to and in registry with the first, the effective K from that environment should oscillate out of phase with P and be tunable in strength through the environment density. Eigenstates of Eq. (8) would then be expected to have the form

$$\vec{\psi}_{n,k}(x) = R(kx)\vec{w}_{n,k}(x), \tag{14}$$

where n is a band index and the function $\vec{w}$ has the periodicity of the monomer pattern. One could then adiabatically vary the twist parameter in $\tilde{H}$ to explore more exotic physics such as the Zak phase [33], but in a classical setting.

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