Dynamical model of Cosserat nanotubes

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Abstract. A Cosserat shell model of a single-wall carbon nanotube is developed based a recent static Cosserat rod model with microstructure. The new dynamical theory is used to study longitudinal acoustic phonon propagation.

Introduction
One of the most attractive features of carbon nanotubes [1] is their exceptional mechanical performance. A carbon nanotube may be considered as a cylinder of graphene and the carbon-carbon bond in graphene is one of the strongest chemical bonds known in nature. Conventional materials have Young’s moduli ranging from a few GPa up to 600 GPa for diamond; the Young’s modulus of a carbon nanotube is typically a few TPa. Thus, recent years have seen a surge of interest in carbon nanotubes with the aim to engineer nano-scale devices.

Calculations of the electronic and mechanical properties of carbon nanotubes often rely on \textit{ab-initio} techniques employing density-functional theory (for example, [2]). However, numerical implementations of such schemes are intensive and can require considerable computing power. Therefore, the dynamical response of carbon nanotubes to external loading is often investigated using effective models based on classical continuum mechanics [3] (for a recent review see [4]). Such approaches require parameters, such as elasticity moduli and mass density, that can be inferred from experimental data or ab-initio quantum calculations [2]. Clearly, one must exercise expediency when formulating an effective theory; there is little gain in developing continuum models that require considerable computing resources when the aim is to efficiently compute the dynamical behaviour of networks of nanotubes.

The Cosserat theory of rods [5] is a powerful and versatile scheme for modelling a large range of slender mechanical continua whose transverse cross-sections do not deform significantly [6]. The theory is capable of effectively describing large deformations from the unstrained reference state and is formulated as a set of coupled non-linear partial differential equations in two independent variables \((s, t)\) for the position and orientation of each cross-section (labelled by \(s \in \mathbb{R}\)) at time \(t\). Evidently, static configurations are especially simple in this picture because they are described by a coupled set of non-linear ordinary (rather than partial) differential equations.

Mechanically deforming a carbon nanotube will lead to changes in the relative positions of the carbon atoms. Bending and twisting the nanotube may lead to significant cross-section deformation, taking the nanotube outside the remit of Cosserat rod theory. Motivated by the efficiency and wide domain of applicability of Cosserat rod theory, a model was recently proposed [7] that describes such cross-section deformation by building extra degrees of freedom onto the basic Cosserat rod model, leading to a “Cosserat tube” (or a “Cosserat rod with
microstructure”). The additional degrees of freedom were motivated by slicing the tube into a finite number of cross-sections, treating each cross-section as a ring-shaped Cosserat rod and taking a limit to the continuum. This procedure led to a static theory that successfully described equilibria of externally loaded tubes.

The present article elucidates a new Cosserat shell [5] model of nanotubes describing “bulk” dynamics (bending, shearing and torsional oscillations) and “microstructure” dynamics (cross-section deformation). The approach here is based on a dimensional reduction of the action for a 3-dimensional mechanical continuum whose cross-sections only permit in-plane deformations, rather than the “bottom-up” approach used in [7]. A “top down” reduction from a 3-dimensional continuum has been adopted here because it includes kinetic terms consistently from the outset. An interesting consequence of the present approach is that although the action for the unreduced 3-dimensional mechanical continuum is motivated by similar considerations to [7], the potential obtained by reducing the 3-dimensional action is slightly different.

A review of the Cosserat theory of rods is given in Section 1 and includes a discussion of an action principle for a Kirchoff Cosserat rod and its derivation from an action for a 3-dimensional mechanical continuum. This is used in Section 2 to motivate a 3-dimensional action for a Cosserat tube whose walls have constant thickness. Section 3 applies the theory to a tube with a straight cylindrical reference configuration (the unstrained state appropriate for a carbon nanotube) and the various contributions to the reduced potential are examined in Section 4 and compared to the potential in [7]. Section 5 discusses the new theory’s prediction for the speed of longitudinal acoustic phonon propagation along the axis of a (10, 10) armchair carbon nanotube.

1. Action principle for a Cosserat rod

A continuum’s mechanical response to deformation is specified relative to one of its static states (the reference configuration). The reference configuration is the static equilibrium state adopted by the continuum in the absence of external forces and torques. In the following, maps evaluated in the reference configuration are distinguished using a circumflex.

The dependent variables describing a Cosserat rod of reference length \( L \) are the positions and orientations of its cross-sections. The position of cross-section \( s \) at time \( t \) is \( r_t(s) \) where \( r_t \) is a space-curve,

\[
r_t : [0, L] \subset \mathbb{R} \rightarrow \mathbb{R}^3
\]

and the \( t \)-dependent orthonormal directors \( (d_1, d_2, d_3 = d_1 \times d_2) \) over \( r_t \) specify the orientations of the cross-sections. Each material point in the rod is labelled by the co-moving coordinates \( (s, \zeta_1, \zeta_2) \) where the pair \( (d_1(s,t), d_2(s,t)) \) span the cross-section labelled by \( s \). The positions of the material points are given by the map \( \Psi \) where

\[
\Psi(s, \zeta_1, \zeta_2, t) = r(s,t) + \zeta_1 d_1(s,t) + \zeta_2 d_2(s,t).
\]

The positions of the material points in the reference configuration are given by \( \hat{\Psi} \) where

\[
\hat{\Psi}(s, \zeta_1, \zeta_2) = \hat{r}(s) + \zeta_1 \hat{d}_1(s) + \zeta_2 \hat{d}_2(s),
\]

\[
\partial_s \hat{r} = \hat{d}_3 = \hat{d}_1 \times \hat{d}_2
\]

and \( s \) is the arc parameter of \( \hat{r} \).

The reference mass density \( \hat{\rho}(s) \) is assumed constant across the reference state \( \hat{C}(s) \) of cross-section \( s \) and \( r \) may be chosen so that

\[
r(s,t) = \frac{1}{A(s)} \int_{\hat{C}(s)} \Psi J_{\hat{\Psi}} d\zeta_1 d\zeta_2
\]
the second rank tensor $I$ for all vectors $X$ with (relations is $\alpha, \beta$ where

\[
\begin{bmatrix}
\partial_{x_1} \Psi \cdot e_x & \partial_{x_2} \Psi \cdot e_x \\
\partial_{y_1} \Psi \cdot e_y & \partial_{y_2} \Psi \cdot e_y \\
\partial_{z_1} \Psi \cdot e_z & \partial_{z_2} \Psi \cdot e_z
\end{bmatrix},
\]

(3)

with $(e_x, e_y, e_z)$ an orthonormal inertial (laboratory) frame and the area $\hat{A}(s)$ of $\hat{C}(s)$ is

\[
\hat{A}(s) = \int_{\hat{C}(s)} J_\Psi d\zeta_1 d\zeta_2.
\]

(4)

Using (1) and (2) it follows that the first area moments of the cross-sections vanish,

\[
\int_{\hat{C}(s)} \zeta_\alpha J_\Psi d\zeta_1 d\zeta_2 = 0
\]

(5)

where $\alpha, \beta = 1, 2$. An action principle for an elastic Cosserat rod with Kirchoff constitutive relations is

\[
S_{rod}[r, d_1, d_2, d_3] = \int dt \int_0^L ds \left[ \frac{1}{2} \hat{A} \partial_s r \cdot \partial_s r + \frac{1}{2} \beta I(\omega, \omega)
\right.
\]

\[
- \frac{1}{2} G \hat{A} \partial_s r \cdot (\partial_s r)_\perp - \frac{1}{2} E \hat{A} (\partial_s r \cdot d_3 - 1)^2
\]

\[
- \frac{1}{2} G I(u_\parallel - \bar{u}_\parallel, u_\parallel - \bar{u}_\parallel) - \frac{1}{2} E I(u_\perp - \bar{u}_\perp, u_\perp - \bar{u}_\perp)
\]

(6)

with

\[
(\partial_s r)_\perp = (\partial_s r \cdot d_1) d_1 + (\partial_s r \cdot d_2) d_2
\]

\[
\omega = \sum_{j=1}^3 d_j \times \partial_s d_j,
\]

\[
u = \sum_{j=1}^3 d_j \times \partial_s d_j, \quad \bar{u} = \sum_{j=1}^3 d_j \times \partial_s d_j,
\]

(7)

\[
u_\perp = (u \cdot d_1) d_1 + (u \cdot d_2) d_2, \quad u_\parallel = (u \cdot d_3) d_3,
\]

\[
u_\perp = (\bar{u} \cdot d_1) d_1 + (\bar{u} \cdot d_2) d_2, \quad \bar{u}_\parallel = (\bar{u} \cdot d_3) d_3
\]

where $G$ and $E$ are material constants (shear modulus and Young’s modulus, respectively) and the second rank tensor $I$ is

\[
I(X, Y) = \sum_{\alpha, \beta = 1}^2 \left( \int_{\hat{C}(s)} \zeta_\alpha \zeta_\beta J_\Psi d\zeta_1 d\zeta_2 \right) (X \times d_\alpha) \cdot (Y \times d_\beta)
\]

(8)

for all vectors $X, Y$. Equations of motion for $r$ and $d_\alpha$ are obtained by extremizing $S$ with respect to $r$ and $d_\alpha$ while maintaining $d_j \cdot d_k = \delta_{jk}$ where $j, k = 1, 2, 3$:

\[
\frac{\delta}{\delta r} S_{rod}[r, d_1, d_2, d_3] = 0,
\]

\[
\frac{\delta}{\delta d_j} S_{rod}[r, d_1, d_2, d_3] = 0,
\]

\[
\delta d_j = K \times d_j.
\]
The variational vectors $\delta r$ and $K$ are chosen to vanish at the rod ends $s = 0, s = L$ leading to the equations of motion

$$
\hat{\rho} \ddot{A} \frac{\partial^2 r}{\partial t^2} = \partial_t n,
\partial_t J = \partial_s r \times n + \partial_t m
$$

where the contact force $n$ and contact torque $m$ are given by the Kirchhoff constitutive relations

$$
n = G \hat{A} (\partial_s r)_\perp + E \hat{A} (\partial_s r \cdot d_3 - 1) d_3,
m \cdot d_3 = GI(u_\parallel - \hat{u}_\parallel, d_3),
m \cdot d_\alpha = EI(u_\perp - \hat{u}_\perp, d_\alpha)
$$

and $J$ is the angular momentum per unit length of the rod where $J \cdot X = \hat{\rho} I(\omega, X)$ for any vector $X$.

In the following section, an action principle for a Cosserat tube is motivated by the decomposition (1) of $\Psi$ with the observation that $S_{\text{rod}}$ can be written

$$
S_{\text{rod}}[r, d_1, d_2, d_3] = \int dt \int_0^L ds \int_{\mathcal{C}(s)} J_\Phi d\varsigma_1 d\varsigma_2 \left[ \frac{1}{2} \hat{\rho} \partial_t \Psi \cdot \partial_t \Psi - \frac{1}{2} G(\partial_s \Psi \cdot d_1 - \partial_s \hat{\Psi} \cdot \hat{d}_1)^2 - \frac{1}{2} G(\partial_s \Psi \cdot d_2 - \partial_s \hat{\Psi} \cdot \hat{d}_2)^2 - \frac{1}{2} E(\partial_s \Psi \cdot d_3 - \partial_s \hat{\Psi} \cdot \hat{d}_3)^2 \right]
$$

where equality with (6) is obtained using (1-5), (7) and (8).

2. Action principle for a Cosserat tube

A material point in the tube is labelled by the triple $(s, \sigma, \zeta)$ and its position at time $t$ is given by $\Phi$,

$$
\Phi(s, \sigma, \zeta, t) = r(s, t) + \xi(s, \sigma, t) + \zeta \mathbf{d}_{(m)}(s, \sigma, t)
$$

with

$$
\xi(s, \sigma, t) = \xi_1(s, \sigma, t) d_1(s, t) + \xi_2(s, \sigma, t) d_2(s, t)
$$

where, like the rod, for simplicity the tube is described using planar cross-sections and the microstructure director $\mathbf{d}_{(m)}$ is constrained to lie in the $(d_1, d_2)$ plane, i.e. $d_3 \cdot \mathbf{d}_{(m)} = 0$ (see Figure 1). At time $t$, cross-section $s$ is located at $r(s, t)$ and its shape is represented by the space-curve $r(s, t) + \xi_{st}$ parametrized by $\sigma$ where $\xi_{st}(\sigma) = \xi(s, \sigma, t)$. Points in the cross-section not located on $r(s, t) + \xi_{st}$ are given by the displacement $\zeta \mathbf{d}_{(m)}(s, \sigma, t)$ with $\zeta \in [\varsigma_1, \varsigma_2]$. The tube’s reference configuration is

$$
\hat{\Phi}(s, \sigma, \zeta) = \hat{r}(s) + \hat{\xi}_1(s, \sigma) \hat{d}_1(s) + \hat{\xi}_2(s, \sigma) \hat{d}_2(s) + \zeta \hat{\mathbf{d}}_{(m)}(s, \sigma)
$$

where $s$ is the arc parameter of $\hat{r}$ and $\sigma$ is the arc parameter of the space-curve $\hat{r}(s) + \hat{\xi}_s$,

$$
\hat{\xi}_s : \sigma \mapsto \hat{\xi}_1(s, \sigma) \hat{d}_1(s) + \hat{\xi}_2(s, \sigma) \hat{d}_2(s),
$$

representing the reference cross-section $\hat{\mathcal{C}}(s)$. The split (11) is chosen so that

$$
\int_{\hat{\mathcal{C}}(s)} \xi_\alpha J_\Phi d\sigma d\zeta = 0
$$
Figure 1. The directors $d_1, d_2, d_{(m)}$ are coloured red and the position vectors $r, r + \xi$ of the space-curves representing the tube’s “bulk” and the cross-section (“microstructure”) are coloured blue. The dashed curves are the two representative space-curves. Note $d_{(m)}$ and $\xi$ lie in the plane spanned by $d_1, d_2$.

and

$$\int_{\hat{\mathcal{C}}(s)} \hat{\zeta} J_{\Phi} d\sigma d\zeta = 0$$

(13)

where $J_{\Phi}$ is the Jacobian of $\hat{\Phi}$,

$$J_{\Phi} = \begin{vmatrix} \partial_s \hat{\Phi} \cdot e_x & \partial_s \hat{\Phi} \cdot e_y & \partial_s \hat{\Phi} \cdot e_z \\ \partial_\zeta \hat{\Phi} \cdot e_x & \partial_\zeta \hat{\Phi} \cdot e_y & \partial_\zeta \hat{\Phi} \cdot e_z \\ \partial_\sigma \hat{\Phi} \cdot e_x & \partial_\sigma \hat{\Phi} \cdot e_y & \partial_\sigma \hat{\Phi} \cdot e_z \end{vmatrix}.$$  

(14)

It follows

$$r(s, t) = \frac{1}{\hat{A}(s)} \int_{\hat{\mathcal{C}}(s)} \Phi J_{\hat{\Phi}} d\sigma d\zeta$$

where $\hat{A}(s)$ is the area of $\hat{\mathcal{C}}(s)$,

$$\hat{A}(s) = \int_{\hat{\mathcal{C}}(s)} J_{\hat{\Phi}} d\sigma d\zeta.$$

Equation (10) suggests that a suitable action principle for a Cosserat tube is
Figure 2. An illustration of the types of deformations associated with the potential terms in (15). (a) The first and second terms are associated with shear along the length of the tube without cross-section deformation. (b) The third term is associated with extension along the length of the tube without cross-section deformation. (c) The fourth term is associated with shearing the cross-sections without longitudinally stretching or bending the tube. (d) The fifth term is associated with dilating the cross-sections without longitudinally stretching or bending the tube.

\[ S_{\text{tube}}[r, d_1, d_2, d_3, \xi_1, \xi_2, d_{(m)}] = \int dt \int \limits_0^L ds \int \limits_{\hat{C}(s)} J_\Phi d\sigma d\zeta \left[ \frac{1}{2} \rho \partial_t \Phi \cdot \partial_t \Phi - \frac{1}{2} G (\partial_s \Phi \cdot d_1 - \partial_s \hat{\Phi} \cdot \hat{d}_1)^2 - \frac{1}{2} G (\partial_s \Phi \cdot d_2 - \partial_s \hat{\Phi} \cdot \hat{d}_2)^2 \\
- \frac{1}{2} G (\partial_s \Phi \cdot d_3 - \partial_s \hat{\Phi} \cdot \hat{d}_3)^2 - \frac{1}{2} G (\partial_\sigma \Phi \cdot d_{(m)} - \partial_\sigma \hat{\Phi} \cdot \hat{d}_{(m)})^2 \\
- \frac{1}{2} E (\partial_\sigma \Phi \cdot d_3 \times d_{(m)} - \partial_\sigma \hat{\Phi} \cdot \hat{d}_3 \times \hat{d}_{(m)})^2 \right] \]

The first three contributions to the potential in \( S_{\text{tube}} \)

\[ \int \limits_0^L ds \int \limits_{\hat{C}(s)} J_\Phi d\sigma d\zeta \left[ \frac{1}{2} G (\partial_s \Phi \cdot d_1 - \partial_s \hat{\Phi} \cdot \hat{d}_1)^2 + \frac{1}{2} G (\partial_s \Phi \cdot d_2 - \partial_s \hat{\Phi} \cdot \hat{d}_2)^2 \\
+ \frac{1}{2} E (\partial_\sigma \Phi \cdot d_3 \times d_{(m)} - \partial_\sigma \hat{\Phi} \cdot \hat{d}_3 \times \hat{d}_{(m)})^2 \right] \]

accommodate “bulk” bending, twisting and shearing and the last two contributions

\[ \int \limits_0^L ds \int \limits_{\hat{C}(s)} J_\Phi d\sigma d\zeta \left[ \frac{1}{2} G (\partial_\sigma \Phi \cdot d_{(m)} - \partial_\sigma \hat{\Phi} \cdot \hat{d}_{(m)})^2 \\
+ \frac{1}{2} E (\partial_\sigma \Phi \cdot d_3 \times d_{(m)} - \partial_\sigma \hat{\Phi} \cdot \hat{d}_3 \times \hat{d}_{(m)})^2 \right] \]
are non-zero when the cross-sections are deformed from their unstrained shapes. The tube material is assumed to be isotropic so extension of the tube and uniform dilation of the cross-sections are described using the same Young’s modulus $E$ (see (b) and (d) in Figure 2). Similarly, shearing the tube transverse to its length without deforming the cross-sections and shearing the cross-sections uniformly along the tube without longitudinal stretch is described using the same shear modulus $G$ (see (a) and (c) in Figure 2).

Equations of motion may be obtained by extremalizing (15) with respect to $r, d_j, \xi_\alpha$ and $d_{(m)}$ subject to the constraints $d_j \cdot d_k = \delta_{jk}, d_3 \cdot d_{(m)} = 0$ and (12) for $j, k = 1, 2, 3$. Alternatively, one may eliminate the constraints on $\xi_\alpha$ and $d_{(m)}$ prior to variation by appropriately parametrizing the microstructure degrees of freedom. The latter approach is used in the following because it permits an easy comparison of the present theory with [7].

3. Cylindrical reference configuration

The reference configuration appropriate for modelling an achiral carbon nanotube [1] is a uniform annular cylinder with radius $R$ and wall thickness $a \ll R$ whose centre lies along the $z$-axis $e_z$ of the orthonormal inertial frame $(e_x, e_y, e_z)$:

\[ \Phi(s, \sigma, \zeta) = \hat{r}(s) + R \left[ \cos \theta \hat{d}_1(s) + \sin \theta \hat{d}_2(s) \right] + \zeta \hat{d}_{(m)}(s, \sigma) \]  

(16)

where

\[ \hat{d}_{(m)}(s, \sigma) = \cos \theta \hat{d}_1(s) + \sin \theta \hat{d}_2(s), \]

(17)

\[ \hat{r} = s e_z, \]

and

\[ (\hat{d}_1, \hat{d}_2, \hat{d}_3) = (e_x, e_y, e_z) \]

(18)

with

\[ \theta = \frac{\sigma}{R} \]

and the area $\hat{A}$ and density $\hat{\rho}$ are constant.

Henceforth, we will use $\theta$ instead of $\sigma$ to locate points around the tube’s cross-sections. For notational simplicity, we will write $d_{(m)}(s, \theta)$ instead of $d_{(m)}(s, R \theta)$ and use this convention for all functions of $\sigma$ introduced thus far.

The cross-sections are conveniently described using the basis

\[ e_{(m)}(s, \theta, t) = \cos \theta d_1(s, t) + \sin \theta d_2(s, t) \]

(19)

\[ d_3(s, t) \times e_{(m)}(s, \theta, t) = -\sin \theta d_1(s, t) + \cos \theta d_2(s, t) \]

where

\[ \hat{e}_{(m)} = \cos \theta \hat{d}_1 + \sin \theta \hat{d}_2 = \cos \theta e_x + \sin \theta e_y, \]

(20)

\[ \hat{d}_3 \times \hat{e}_{(m)} = -\sin \theta \hat{d}_1 + \cos \theta \hat{d}_2 = -\sin \theta e_x + \cos \theta e_y \]

are radial and azimuthal unit vectors in the reference cross-sections. The space-curve

\[ \theta \mapsto \xi(s, \theta, t) = \xi_1(s, \theta, t) d_1(s, t) + \xi_2(s, \theta, t) d_2(s, t) \]

represents cross-section $s$ at time $t$ and $\xi$ is written

\[ \xi(s, \theta, t) = R \left\{ [1 + \gamma(s, \theta, t)] e_{(m)}(s, \theta, t) + \chi(s, \theta, t) d_3(s, t) \times e_{(m)}(s, \theta, t) \right\} \]

(21)

where $\dot{\gamma} = \dot{\chi} = 0$ and

\[ \dot{\xi}(s, \theta) = R \dot{e}_{(m)}(s, \theta) \]

in the reference configuration. The microstructure director $d_{(m)}$ is written

\[ d_{(m)}(s, \theta, t) = \cos \psi(s, \theta, t) e_{(m)}(s, \theta, t) + \sin \psi(s, \theta, t) d_3(s, t) \times e_{(m)}(s, \theta, t) \]

(22)
so
\[ \mathbf{d}_3(s, t) \times \mathbf{d}_m(s, \theta, t) = -\sin \psi(s, \theta, t) \mathbf{e}_m(s, \theta, t) + \cos \psi(s, \theta, t) \mathbf{d}_3(s, t) \times \mathbf{e}_m(s, \theta, t) \]

where \( \hat{\psi} = 0 \) and \( \hat{\mathbf{d}}_m = \hat{\mathbf{e}}_m \) in the reference configuration.

4. The structure of the Cosserat nanotube potential
A comparison between the present model and the model introduced in [7] is made by writing \( \Phi \) in (15) as
\[ \Phi(s, \theta, \zeta, t) = \Xi(s, \theta, t) + \zeta \mathbf{d}_m(s, \theta, t) \]

where
\[ \Xi(s, \theta, t) = r(s, t) + R\{[1 + \gamma(s, \theta, t)] \mathbf{e}_m(s, \theta, t) + \chi(s, \theta, t) \mathbf{d}_3(s, t) \times \mathbf{e}_m(s, \theta, t) \} \]

The potential in (15) naturally splits into the bulk contribution \( W(b) \),
\[ W(b) = \int_0^L ds \int_{C(s)} J_3 \sigma d\zeta \left[ \frac{1}{2} G \left( \partial_\sigma \Phi \cdot \mathbf{d}_1 - \partial_\sigma \hat{\Phi} \cdot \hat{\mathbf{d}}_1 \right)^2 + \frac{1}{2} G \left( \partial_\sigma \Phi \cdot \mathbf{d}_2 - \partial_\sigma \hat{\Phi} \cdot \hat{\mathbf{d}}_2 \right)^2 \right. 
\]
\[ \left. + \frac{1}{2} E \left( \partial_\sigma \Phi \cdot \mathbf{d}_3 - \partial_\sigma \hat{\Phi} \cdot \hat{\mathbf{d}}_3 \right)^2 \right], \]

and the microstructure contribution \( W(m) \),
\[ W(m) = \int_0^L ds \int_{C(s)} J_3 \sigma d\zeta \left[ \frac{1}{2} G \left( \partial_\sigma \Phi \cdot \mathbf{d}_m - \partial_\sigma \hat{\Phi} \cdot \hat{\mathbf{d}}_m \right)^2 \right. 
\]
\[ \left. + \frac{1}{2} E \left( \partial_\sigma \Phi \cdot \mathbf{d}_3 \times \mathbf{d}_m - \partial_\sigma \hat{\Phi} \cdot \hat{\mathbf{d}}_3 \times \hat{\mathbf{d}}_m \right)^2 \right]. \]

The integrals (24) and (25) are of the form
\[ \Lambda(t) = \int_{\mathcal{C}(s)} J_3 \sigma d\zeta \left[ \mathfrak{A}(s, \theta, t) + \mathfrak{B}(s, \theta, t) \zeta + \mathfrak{C}(s, \theta, t) \zeta^2 \right] \]

and using (14), (16), (17) it follows \( J_3 = 1 + \zeta / R \) is independent of \( \theta \) and
\[ \Lambda = \int_0^{2\pi} d\theta \int_{\zeta_1}^{\zeta_2} (R + \zeta) (\mathfrak{A} + \mathfrak{B} \zeta + \mathfrak{C} \zeta^2) d\zeta \]
\[ = \int_0^{2\pi} \left( \frac{1}{2\pi} \tilde{\mathfrak{A}} + \frac{1}{2\pi} \tilde{\mathfrak{B}} \zeta \right) d\theta \]

where
\[ \tilde{\mathfrak{A}} = \int_{\mathcal{C}(s)} J_3 \sigma d\zeta = 2\pi \int_{\zeta_1}^{\zeta_2} (R + \zeta) d\zeta, \]
\[ \tilde{\mathfrak{B}} = \int_{\mathcal{C}(s)} J_3 \zeta^2 d\sigma d\zeta = 2\pi \int_{\zeta_1}^{\zeta_2} (R + \zeta) \zeta^2 d\zeta \]

with \( \zeta_1 = R_1 - R, \zeta_2 = R_2 - R \) where \( R_1, R_2 \) are the inner and outer radii of the tube’s reference state. The terms containing \( \mathfrak{B} \) in (26) vanish as a consequence of (13):
\[ \int_{\mathcal{C}(s)} J_3 \zeta d\sigma d\zeta = 0 \]
\[ = 2\pi \int_{\zeta_1}^{\zeta_2} (R + \zeta) \zeta d\zeta \]
leading to an algebraic relationship between \( R, R_1 \) and \( R_2 \). Eliminating \( R_2 \) in terms of \( R \) and \( R_1 \) in \( \hat{A} \) and \( \hat{I} \) and using \( R_1 = R[1 + O(a/R)] \) yields

\[
\hat{A} = 2\pi Ra \left[ 1 + O \left( \frac{a}{R} \right) \right],
\]
\[
\hat{I} = \frac{\pi}{6} Ra^3 \left[ 1 + O \left( \frac{a}{R} \right) \right].
\]  

Using (17), (20), (23) and \( \hat{\gamma} = \hat{\chi} = 0 \) it follows \( \partial s \hat{\Xi} = \hat{e}_z = \hat{d}_3 \). Furthermore, \( \hat{d}_{(m)} = \hat{e}_{(m)} \) so \( \partial s \hat{d}_{(m)} = 0 \) and using (27) and (24) the bulk potential \( W_{(b)} \) is

\[
W_{(b)} = \int_0^L ds \int_0^{2\pi} d\theta \left[ \frac{1}{4\pi} G \hat{A} (\partial_s \Xi)_\perp \cdot (\partial_s \Xi)_\perp + \frac{1}{4\pi} E \hat{A} (\partial_s \Xi \cdot d_3 - 1)^2 
+ \frac{1}{4\pi} G \hat{I} (\partial_s d_{(m)})_\perp \cdot (\partial_s d_{(m)})_\perp + \frac{1}{4\pi} E \hat{I} (\partial_s d_{(m)} \cdot d_3)^2 \right]
\]  

where

\[
(\partial_s \Xi)_\perp = (\partial_s \Xi \cdot d_1) d_1 + (\partial_s \Xi \cdot d_2) d_2, \quad (\partial_s d_{(m)})_\perp = (\partial_s d_{(m)} \cdot d_1) d_1 + (\partial_s d_{(m)} \cdot d_2) d_2.
\]

Using (19) and

\[
d_1 = d_2 \times d_3, \quad d_2 = d_3 \times d_1, \quad d_3 = d_1 \times d_2
\]

it follows

\[
\partial_s \Phi \cdot d_{(m)} = (\partial_\theta \gamma - \chi) \cos \psi + (1 + \gamma + \partial_\theta \chi) \sin \psi,
\]
\[
\partial_s \Phi \cdot d_3 \times d_{(m)} = - (\partial_\theta \gamma - \chi) \sin \psi + (1 + \gamma + \partial_\theta \chi) \cos \psi + \frac{\zeta}{R} (\partial_\theta \psi + 1)
\]  

and since \( \hat{\gamma} = \hat{\chi} = \hat{\psi} = 0 \),

\[
\partial_s \Phi \cdot d_{(m)} = 0,
\]
\[
\partial_s \Phi \cdot d_3 \times d_{(m)} = 1 + \frac{\zeta}{R}.
\]  

Using (27), (31) and (32) to express the microstructure potential \( W_{(m)} \) (25) in terms of \( \gamma, \chi, \psi \) leads to

\[
W_{(m)} = \int_0^L ds \int_0^{2\pi} d\theta \left\{ \frac{1}{4\pi} G \hat{A} [(\partial_\theta \gamma - \chi) \cos \psi + (1 + \gamma + \partial_\theta \chi) \sin \psi]^2 
+ \frac{1}{4\pi} E \hat{A} [-(\partial_\theta \gamma - \chi) \sin \psi + (1 + \gamma + \partial_\theta \chi) \cos \psi - 1]^2 
+ \frac{1}{4\pi} E \hat{I} (\partial_\theta \psi)^2 \right\}.
\]

The decomposition (11) is fixed using (12) and since \( \xi_\alpha \) is independent of \( \zeta \) it follows

\[
\int_0^{2\pi} \frac{1}{2\pi} \hat{A} \xi_\alpha (s, \theta, t) d\theta = 0
\]  

where (27) has been used. Equations (34), (21), (19) and \( \xi_\alpha = \xi \cdot d_\alpha \) lead to

\[
\int_0^{2\pi} (\gamma \cos \theta - \chi \sin \theta) d\theta = 0,
\]
\[
\int_0^{2\pi} (\gamma \sin \theta + \chi \cos \theta) d\theta = 0
\]  

i.e. the first Fourier modes of \( \gamma \) and \( \chi \) in \( \theta \) are not independent.

The microstructure potential introduced in [7] is recovered from (33) for small deformations from \( \hat{\gamma} = \hat{\chi} = \hat{\psi} = 0 \). In this case \( \gamma, \chi, \psi \) and their first derivatives are small and it follows

\[
W_{(m)} \simeq \int_0^L ds \int_0^{2\pi} d\theta \left[ \frac{1}{4\pi} G A \left( \partial_\theta \gamma - \chi + \psi \right)^2 + \frac{1}{4\pi} E \hat{A} \left( \gamma + \partial_\theta \chi \right)^2 + \frac{1}{4\pi} \frac{E \hat{T}}{R^2} \left( \partial_\theta \psi \right)^2 \right]
\]

which, using (29), yields equation (16) in [7].

The bulk potential \( W_{(b)} \) couples the cross-sections in a slightly different way to the model explored in [7]. The model in [7] is developed using a potential of the form

\[
W(I) = \int_0^L ds \int_0^{2\pi} d\theta \left[ \frac{1}{4\pi} G \hat{A} \left( \partial_s \Xi \right)_\perp \cdot \left( \partial_s \Xi \right)_\perp + \frac{1}{4\pi} E \hat{A} \left( \partial_s \Xi \cdot d_3 - 1 \right)^2 \right] + W_{(m)}
\]

whereas the potential \( W_{(II)} = W_{(b)} + W_{(m)} \) in the model discussed here includes \( W(I) \) and an additional coupling between the cross-sections:

\[
W_{(II)} = W_{(I)} + \int_0^L ds \int_0^{2\pi} d\theta \left[ \frac{1}{4\pi} G \hat{T} \left( \partial_s d_{(m)} \right)_\perp \cdot \left( \partial_s d_{(m)} \right)_\perp + \frac{1}{4\pi} E \hat{T} \left( \partial_s d_{(m)} \cdot d_3 \right)^2 \right].
\]

5. Longitudinal acoustic phonon propagation and the \( A_{1g} \) radial breathing mode

A simple set of differential equations generated using (15) describe azimuthally symmetric motion (dilation and extension) of a straight tube. This system is readily obtained by setting almost all dependent degrees of freedom equal to their reference values in (15) prior to variation.

Substituting \( r = Z(s, t) e_z, \psi = \hat{\psi} = 0, \chi = \hat{\chi} = 0 \), suppressing the \( \theta \) dependence of \( \gamma \) and setting \( (d_1, d_2, d_3) = (\hat{d}_1, \hat{d}_2, \hat{d}_3) \) yields

\[
S_{\text{tube}}[Z, \gamma] = \int dt \int_0^L ds \left\{ \frac{1}{2} \hat{\rho} \hat{A} \left( \partial_t Z \right)^2 + R^2 \left( \partial_t \gamma \right)^2 \right\} - \frac{1}{2} GAR^2 \left( \partial_s \gamma \right)^2 - \frac{1}{2} E \hat{A} \left( \partial_s Z - 1 \right)^2 - \frac{1}{2} E \hat{A} \gamma^2 \right\}
\]

and the constraints (35) are automatically satisfied. There are no terms in (37) coupling \( \gamma \) and \( Z \) together so such longitudinal and radial deformations are decoupled.

Extremalizing (37) with respect to \( Z \) and \( \gamma \),

\[
\frac{\delta}{\delta Z} S_{\text{tube}}[Z, \gamma] \equiv 0,
\]
\[
\frac{\delta}{\delta \gamma} S_{\text{tube}}[Z, \gamma] \equiv 0
\]

subject to variations \( \delta Z \) and \( \delta \gamma \) that vanish at \( s = 0 \) and \( s = L \) leads to

\[
\hat{\rho} \hat{A} \partial_t^2 Z - E \hat{A} \partial_t^2 Z = 0,
\]
\[
\hat{\rho} \hat{AR}^2 \partial_t^2 \gamma - GAR^2 \partial_s^2 \gamma + E \hat{A} \gamma = 0.
\]

1 There is an erroneous factor of \( \pi \) multiplying (16) in [7].
Thus, disturbances in the extension of the tube travel with the phase speed $c_s$, 

$$c_s = \sqrt{\frac{E}{\bar{\rho}}}, \quad (38)$$

whereas dilation waves are dispersive and satisfy 

$$\omega(k) = \sqrt{\frac{G}{\bar{\rho} k^2} + \frac{E}{\bar{\rho} R^2}} \quad (39)$$

where $\gamma = a \cos(ks - \omega t)$. Using (38) and (39) it follows 

$$c_s = \omega_0 R \quad (40)$$

where $\omega_0 = \omega(0)$ is the angular frequency of the fundamental radial breathing mode $k = 0$.

For an armchair $(10,10)$ carbon nanotube $R = 6.785 \text{ Å}$ and Raman spectroscopy yields $\lambda^{-1} = 165 \text{ cm}^{-1}$ where the angular frequency of the $A_{1g}$ breathing mode is $\omega_0 = 2\pi c \lambda^{-1}$ and $c$ is the speed of light in the vacuum [1]. Thus, (40) leads to $c_s = 21.08 \text{ km/s}$ which compares favourably with typical phase speeds for longitudinal acoustic (LA) phonons (e.g. $c_s = 20.35 \text{ km/s}$ [1]).

**Conclusion**

A dynamical Cosserat shell model of a single-wall carbon nanotube has been presented and some of its properties discussed. It was obtained from a reduction of an action for a 3-dimensional tube whose wall thickness is constant and it was shown that the new model includes the potential terms used in [7] and additional couplings between the cross-sections. The model predicts that longitudinal acoustic phonons in type $(10,10)$ carbon nanotubes propagate at a speed that agrees satisfactorily with experimental data.

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