Optimal Functions and Nanomechanics III

APP MTH 3022/7106

Barry Cox

Lecture 24

Last lecture

- Defined what we mean by line curvature
- Derived an expression for the curvature

$$\kappa = \sqrt{\ddot{x}^2 + \ddot{y}^2} = \frac{y''}{(1 + y'^2)^{3/2}}$$

- Reviewed the history of the elastica
- Solved a "simple" elastica problem with no length constraint

Joining nanostructures

We would like to know how a carbon nanotube might join to a graphene sheet. This will help understand the requirements of constructing nano-electro-mechanical systems assembled from these building-blocks.

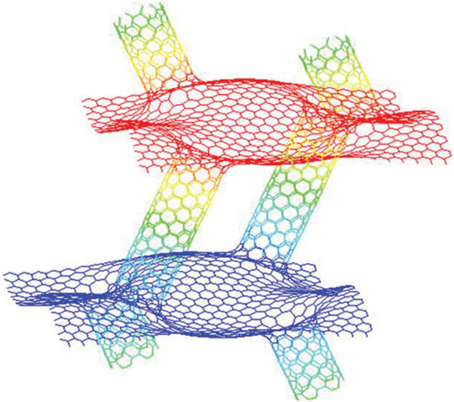


Figure: Dr Ajit Roy

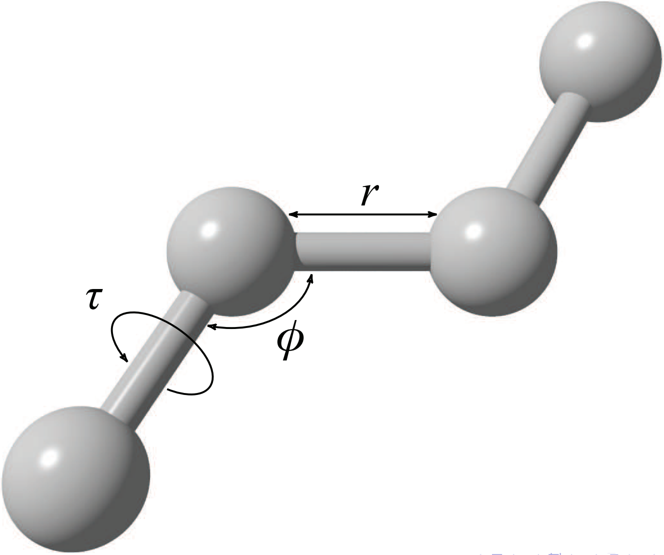
Models

It make sense that the shape of the join region would be dictated by energy considerations. One model for the energy of perturbed chemical bonds is

$$E = \frac{1}{2}\sum_{i,j}\left\{k_r(r_{ij}-r_0)^2 + k_\phi(\phi_{ij}-\phi_0)^2 + k_\tau\left[1 - cos(n\tau_{ij}-\tau_0)\right]\right\}.$$

where i, j iterates over all the bonded atoms, with r_{ij}, ϕ_{ij} and τ_{ij} are the bond length, bond angle and bond torsion, respectively. The corresponding terms with subscript 0 denote the ideal values for these quantities (the unperturbed bond length, angle and torsion) and k_r, k_ϕ and k_τ are weightings for the various modes of perturbation to the chemical bond. Finally n relates to the periodicity of the chemical bond.

Models



Models

So one approach is to calculate E by brute force from all the atomic positions and then minimise the energy using standard optimisation techniques.

Another idea would be to assume the chemical bonds participating in the joing region are behaving like an elastic material with different elastic moduli given by k_r, k_ϕ and k_τ. And in general the moduli are such that

$$k_r \gg k_\phi \gg k_\tau.$$

Since to join say a graphene sheet to a nanotube we know we need to perturb ϕ we can assume that $r_i = r_0$, $\forall i$ and further we might assume that the k_τ contribution is negligible.

Rather like the elastica

However if wanted to do a continuum model we might say well this is sounding a lot like the elastica.

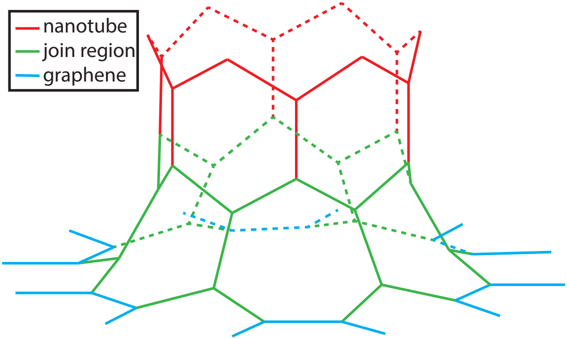
Fixing all bond lengths to the ideal value r_0 is equivalent to setting a isoperimetric constraint on the join length.

The weight of the nanostructure is negligible due to the scale of the problem.

So we can propose a model where the shape of the join region will be approximately the shape of an appropriately constrained elastica.

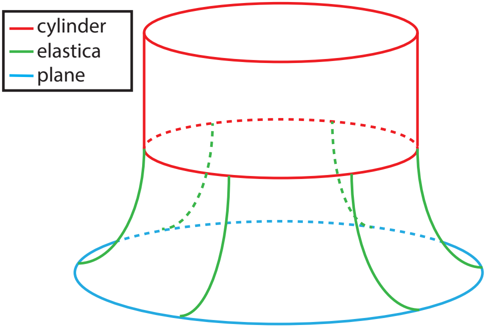
Perpendicular joining of nanotube and graphene

We assume the elastic energy is given by the line curvature squared of the joining covalent bonds. Then we have a fixed length constraint on the join region minimising κ^2 and the starting point is fixed in position and derivative but the end point only has a fixed derivative.



Idealised model

We assume the graphene is a flat plane with a circular hole; the nanotube is a cylinder with perpendicular orientation to the plane and the join region comprises thin elastic rods, or elastica.



Physical parameters

We have a nanotube with radius a and a defect in the graphene plane that we assume to be a circle with radius R. Let's denote the difference by $x_1 = R - a$.

We also have the elastica which we will take to be fixed with length L.

So out end-point conditions will be

$$y(0) = 0, \quad y'(0) = 0, \quad y'(x_1) \to \infty.$$

The value of $y(x_1) = y_1$ is not specified and we will determine this from the natural boundary condition on that end-point.

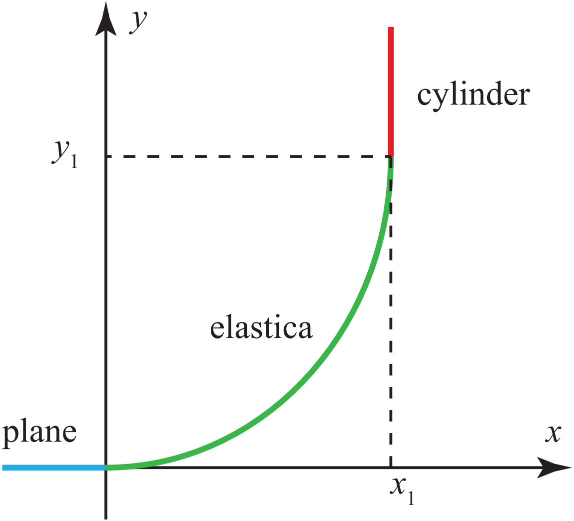
Problem geometry

Endpoint conditions

$$\begin{aligned} y(0) &= 0 \\ y'(0) &= 0 \\ y(x_1) &= y_1 \\ y'(x_1) &\to \infty \end{aligned}$$

Remember that x_1 is prescribed as part of the problem.

However we need to find y_1 as part of the solution.



Functional and length constraint

So the functional we are minimising is κ^2 but we also have a length constraint which we need to add with a Lagrange multiplier. That is

$$
\begin{aligned}
F\{y\} &= \int_0^L \kappa^2\, ds + \lambda \int_0^L \, ds \\
&= \int_0^{x_1} \left(\frac{y''^2}{(1+y'^2)^3} + \lambda \right) (1+y'^2)^{1/2} dx \\
&= \int_0^{x_1} \left[\frac{y''^2}{(1+y'^2)^{5/2}} + \lambda (1+y'^2)^{1/2} \right] dx.
\end{aligned}
$$

We also have the constraint itself which we will use to determine the value of one of our arbitrary constants

$$
\int_0^{x_1} (1+y'^2)^{1/2} dx = L.
$$

Natural boundary condition

There is no variation at the $x = 0$ end-point since the position and derivative are prescribed. However at $x = x_1$ we are prescribing the derivative but not the position and so our choice for η will include functions which vanish at $x = 0$ and whose derivative vanishes at $x = 0$ and $x = x_1$. Recall that in deriving the first variation we generated the end-point terms

$$\delta F = \left[\eta\left(\frac{\partial f}{\partial y'} - \frac{d}{dx}\frac{\partial f}{\partial y''}\right) + \eta'\frac{\partial f}{\partial y''}\right]_0^{x_1} + \int \cdots$$

Since η does not necessarily vanish at $x = x_1$, the natural boundary condition requires that

$$\left.\left(\frac{\partial f}{\partial y'} - \frac{d}{dx}\frac{\partial f}{\partial y''}\right)\right|_{x=x_1} = 0$$

Euler-Poisson Equations

Roughly following the working from the last lecture we have the general Euler-Poisson equations

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} = 0.$$

Again since our integrand f is independent of y we can integrate once to yield

$$\frac{\partial f}{\partial y'} - \frac{d}{dx}\frac{\partial f}{\partial y''} = \alpha.$$

However this time we know this must be true for $0 \leqslant x \leqslant x_1$ and the natural boundary condition says the LHS vanishes at $x = x_1$ and therefore $\alpha \equiv 0$.

General result

So picking up from the general result from the last lecture with the additional information that $\alpha = 0$ for this problem we have

$$f - y'' \frac{\partial f}{\partial y''} = -\beta.$$

Now we have to substitute our f and so we have

$$\begin{aligned} \frac{y''^2}{(1+y'^2)^{5/2}} + \lambda(1+y'^2)^{1/2} - y'' \left(\frac{2y''}{(1+y'^2)^{5/2}} \right) &= -\beta \\ -\frac{y''^2}{(1+y'^2)^{5/2}} + \lambda(1+y'^2)^{1/2} &= -\beta \\ \frac{y''^2}{(1+y'^2)^3} &= \lambda + \frac{\beta}{(1+y'^2)^{1/2}} \end{aligned}$$

Curvature equation

So in other words we have derived an expression for the curvature which this time is

$$\kappa = \left(\lambda + \frac{\beta}{(1 + y'^2)^{1/2}} \right)^{1/2}.$$

Following the working from last lecture we again assume $\kappa > 0$ and make the substitution $y' = \tan\theta$. Making this substitution the above equation becomes

$$\kappa = (\lambda + \beta \cos\theta)^{1/2}.$$

Parametric system of DEs

As before we consider x and y to be functions of the parameter θ and so we have the equations

$$\frac{dx}{d\theta} = \frac{\cos\theta}{(\lambda + \beta\cos\theta)^{1/2}},$$
$$\frac{dy}{d\theta} = \frac{\sin\theta}{(\lambda + \beta\cos\theta)^{1/2}}.$$

Again to simplify we are going to redefine our constants and parameter. First we define

$$k = \left(\frac{\lambda + \beta}{2\beta}\right)^{1/2} \quad \text{and} \quad \gamma = \left(\frac{2}{\beta}\right)^{1/2}.$$

New parameter: ϕ

Our new parameter ϕ will be defined by the relationship

$$k \sin \phi = \sin \frac{\theta}{2}.$$

From this we may deduce that

$$\cos \theta = 1 - 2k^2 \sin^2 \phi, \quad \sin \theta = 2k \sin \phi (1 - k^2 \sin^2 \phi)^{1/2}.$$

from which we have

$$\frac{d\theta}{d\phi} = \frac{2k \cos \phi}{(1 - k^2 \sin^2 \phi)^{1/2}},$$

New parameter: ϕ

On substitution, the change of parameter gives

$$\lambda + \beta\cos\theta = \lambda + \beta(1 - 2k^2\sin^2\phi) = 2\beta\left(\frac{\lambda+\beta}{2\beta} - k^2\sin^2\phi\right)$$
$$= 4\frac{k^2}{\gamma^2}(1 - \sin^2\phi)$$
$$(\lambda + \beta\cos\theta)^{1/2} = 2\frac{k}{\gamma}\cos\phi.$$

So

$$\frac{dx}{d\phi} = \frac{dx}{d\theta}\frac{d\theta}{d\phi} = \left(\frac{1 - 2k^2\sin^2\phi}{2\frac{k}{\gamma}\cos\phi}\right)\frac{2k\cos\phi}{(1 - k^2\sin^2\phi)^{1/2}},$$
$$= \gamma\frac{1 - 2k^2\sin^2\phi}{\left(1 - k^2\sin^2\phi\right)^{1/2}},$$

New parameter: ϕ

Likewise

$$\frac{dy}{d\phi} = \frac{dy}{d\theta}\frac{d\theta}{d\phi} = \left(\frac{2k\sin\phi(1-k^2\sin^2\phi)^{1/2}}{2\frac{k}{\gamma}\cos\phi}\right)\frac{2k\cos\phi}{(1-k^2\sin^2\phi)^{1/2}},$$
$$= 2\gamma k\sin\phi.$$

So our relatively complicated equations have reduced to

$$\frac{dx}{d\phi} = \gamma\frac{1-2k^2\sin^2\phi}{\left(1-k^2\sin^2\phi\right)^{1/2}},$$
$$\frac{dy}{d\phi} = 2\gamma k\sin\phi.$$

Solution

So whereas $0 \leqslant \theta \leqslant \pi/2$ we now have $0 \leqslant \phi \leqslant \phi_1$ where $\phi_1 = \sin^{-1}(1/\sqrt{2}k)$. Integrating the y equation is straightforward and since $y(0) = 0$ we have

$$y(\phi) = 2\gamma k \left(1 - \cos\phi\right).$$

The x equation is more work but similar to our previous elastica example we can write the x equation as

$$\frac{dx}{d\phi} = \gamma \left[2\left(1 - k^2 \sin^2\phi\right)^{1/2} - \frac{1}{\left(1 - k^2 \sin^2\phi\right)^{1/2}} \right],$$

which we now recognise as elliptic integrals and therefore

$$x(\phi) = \gamma \left[2E(\phi, k) - F(\phi, k)\right],$$

noting that we have used $x(0) = 0$.

Determining the constants

We still need to determine two constants γ and k. We have one end-point condition we haven't used yet, namely

$$x(\phi_1) = x_1 = \gamma \left[2E(\phi_1, k) - F(\phi_1, k) \right].$$

For another we have to examine the length constraint. Recall this was

$$\int_0^{x_1} (1 + y'^2)^{1/2} dx = L.$$

Making the substitution $y' = \tan\theta$ we have

$$\int_0^{\pi/2} \frac{d\theta}{(\lambda + \beta\cos\theta)^{1/2}} = L.$$

Determining the constants

Getting the length constraint into the new parameter ϕ and constants we have

$$\gamma \int_0^{\phi_1} \frac{d\phi}{(1 - k^2 \sin^2 \phi)^{1/2}} = L,$$

and therefore

$$L = \gamma F(\phi_1, k).$$

This provides us a second equation which means we can in principle determine the two arbitrary constants γ and k and therefore find the unique solution.

Non-dimensional parameter: μ

To simplify the task we consider the quantity

$$\mu = \frac{x_1}{L} = \frac{\gamma\left[2E(\phi_1, k) - F(\phi_1, k)\right]}{\gamma F(\phi_1, k)} = 2\frac{E(\phi_1, k)}{F(\phi_1, k)} - 1.$$

μ is prescribed in the problem and this relation depends only on k (not γ) and from physical considerations we note $-1 < \mu < 1$.

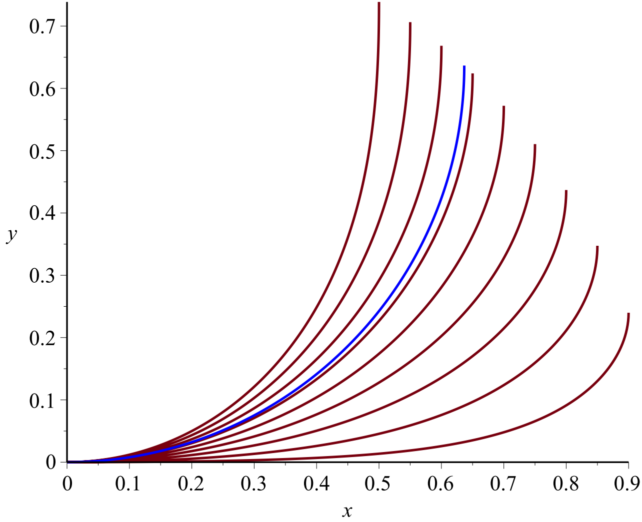
So the way to solve for these constants is to compute $\mu = x_1/L$. From this we can numerically solve this transcendental equation for k. Once k is known we can then use either formula

$$\gamma = \frac{x_1}{2E(\phi_1, k) - F(\phi_1, k)}, \quad \text{or} \quad \gamma = \frac{L}{F(\phi_1, k)}$$

to immediately resolve the last unknown and therefore we can find y_1 from

$$y_1 = 2\gamma k\left(1 - \cos\phi_1\right).$$

Plot of the solutions for $L = 1$



The quarter-circle (blue) is a part of this family of elastica and corresponds to $\mu = 2/\pi$. So Jordanus' guess was correct in this case.

Note: we don't plot values of $\mu < 0.5$

What about $\mu < 0.5$?

Looking at the plot we see the curvature for the $\mu = 0.5$ curve is getting very close to zero (zero curvature = straight line).

At around $\mu = 0.5$ the curvature changes sign and so our earlier assumption of strictly positive curvature breaks down.

We can handle the change in curvature but it must be done carefully and it requires more work.

So we will ignore this case for now.

Are the $\gamma, k, \phi_1 \in \mathbb{R}$?

Sometimes but not always.

For the plot show the curves less than the quarter-circle ($\mu < 2/\pi$) they are all real. However there is a degeneracy at $\mu = 2/\pi$ and for values greater than this critical value all three constants are purely imaginary.

However this does not present a problem provided we constrain our parameter ϕ to remain on the imaginary axis, we can plot the solutions because $x(\phi)$ and $y(\phi)$ remain real.

However it is worth noting that care must be taken in handling these solution with a numerical engine. Since if you make the assumption that you constants must be real you would miss out on a whole branch of the possible solutions.

Speaking of numerical care

It's also worth mentioning that not everyone agrees about the best way to define the elliptic integrals. We've been using

$$F(\phi, k) = \int_0^\phi \frac{d\varphi}{\sqrt{1 - k^2 \sin^2 \varphi}}.$$

However, MAPLE uses

$$\mathrm{EllipticF}(z, k) = \int_0^z \frac{d\zeta}{\sqrt{(1 - \zeta^2)(1 - k^2\zeta^2)}}.$$

So in MAPLE you will need to type something like

```
> EllipticF(sin(phi),k);
```

Speaking of numerical care

MatLab uses

$$\text{ellipticF}(\phi, m) = \int_0^\phi \frac{d\varphi}{\sqrt{1 - m\sin^2\varphi}}.$$

and so you would need to enter

```
> ellipticF(phi,k^2)
```

While Mathematica (Wolfram) uses the similar

$$\text{EllipticF}(\phi, m) = \int_0^\phi \frac{d\varphi}{\sqrt{1 - m\sin^2\varphi}}.$$

and so the Mathematica syntax it would be

```
In[1]:= EllipticF[phi,k^2]
```

And if you are using some other numerical package you will have to check which definition of the elliptic integrals they have implemented.