School of Mathematical Sciences

APP MTH 3022 - Optimal Functions and Nanomechanics III

Tutorial 4 (Week 8)

1. Assuming an interaction potential of the form $\Phi(\rho) = -A\rho^{-6} + B\rho^{-12}$, calculate an analytic expression for the interaction of
   (a) A point $P = (0, 0, \delta)$ and a line ℓ_1 collinear with the x-axis, $-\infty < x < \infty$, assuming a uniform line density of η_1.
   (b) The line ℓ_1 from part (a) and a second line ℓ_2 given by $(t\cos\theta, t\sin\theta, \delta)$ where θ and δ are fixed and the line is parameterised by the variable $-\infty < t < \infty$, assuming a line density of η_2 for ℓ_2
   (c) What is the interaction between ℓ_1 and ℓ_2 in the case of $\theta = \pi/2$?
   (d) What is the interaction between ℓ_1 and ℓ_2 in the case of $\theta = \pi$?

2. A toroidal surface $\mathcal{T}$ may be specified parametrically by its position vector given by

$$\boldsymbol{r}(\theta, \phi) = ((R + r\cos\theta)\cos\phi, (R + r\cos\theta)\sin\phi, r\sin\theta),$$

   where r is the radius of the tube and R is the distance from the centre of the torus to the centre of the tube, and $-\pi < \theta \leqslant \pi, -\pi < \phi \leqslant \pi$.
   (a) Calculate the tangent vector in the θ-direction.
   (b) Calculate the tangent vector in the ϕ-direction.
   (c) Using your answers from parts (a) and (b) determine the scalar area element $\mathrm{d}A$ for $\mathcal{T}$.
   (d) Hence derive an expression for the surface area of $\mathcal{T}$.

3. (a) $\star$ Employing the Lennard-Jones potential and the continuum approximation, derive an explicit expression for the interaction between a nanotorus defined by the surface $\mathcal{T}$ from Q2 and an atom located at the origin.
   (b) $\star$ Using your expression from part (a), compute the numerical value of the interaction energy assuming a nanotorus with $r = 5$ Å and $R = 15$ Å, and a surface density of $\eta = 0.3812$ atoms·Å^{-2} using values of $A = 17.4$ eV·Å^6 and $B = 29\,000$ eV·Å^{12}.
   (c) $\star$ Using the values of parameters from part (b) but allowing R to take on any positive value $R > r$, compute the value of R that leads to a global minimum in the interaction energy for the atom-nanotorus system.

4. Use Ritz's method to find an approximate solution to minimize the

$$J\{y\} = \int_0^{2\pi} \left(y'^2 + \lambda^2 y^2\right)\, dx,$$

   where $y(0) = 1$ and $y(2\pi) = 1$ and λ is a positive integer. Use the trial functions

$$\phi_0 = 1, \quad \phi_n(x) = \sin[(n - 1/2)x].$$

   and so

$$y_N = \phi_0 + \sum_{n=1}^{N} c_n \phi_n(x).$$

   Compare your solution to one found directly from the Euler-Lagrange equations.