PCS 2020-21 exam – problem

I) Entanglement length and tube radius

1.1) κ is the bending rigidity of the polymer. The κ term expresses the energy cost of curving the filament.

1.2) ℓ_p is the polymer's persistence length. It is the typical distance over which a freely floating filament subjected to thermal fluctuation bends, or equivalently the distance over which its initial orientation is lost.

1.3)
$$E = \int_{-\infty}^{+\infty} \frac{\kappa q^4 + \sigma q^2 + \lambda}{2} \underbrace{|\tilde{U}(q)|^2}_{= \tilde{U}_x^2(q) + \tilde{U}_y^2(q)} \frac{dq}{2\pi}$$

1.4) E is a sum of independent harmonic degrees of freedom (almost). The average energy of each must be $\frac{k_B T}{2}$ per the equipartition theorem:

$$\left\langle \frac{\kappa q^4 + \sigma q^2 + \lambda}{2} \tilde{U}_x(q) \tilde{U}_x(q') \right\rangle = \frac{k_B T}{2} \delta_{qq'}$$

$\delta_{qq'}$ goes to $2\pi\delta(q+q')$ in the c^{uum} limit (must give 1 when integrated over q')

and $\langle \tilde{U}_x(q) \tilde{U}_y(q') \rangle = 0$ (indpt degrees of freedom).

So
$$\langle \tilde{U}_i(q) \tilde{U}_j(q') \rangle = \frac{k_B T}{\kappa q^4 + \sigma q^2 + \lambda} \delta_{ij} \, 2\pi \delta(q+q')$$

Thus $\underline{H(q) = \kappa q^4 + \lambda}$

1.5) $$\langle U_x^2(0)\rangle = \left\langle \left(\int_{-\infty}^{+\infty} \tilde{U}_x(q)\,\frac{dq}{2\pi}\right)^2 \right\rangle$$

$$= \iint \frac{dq}{2\pi}\frac{dq'}{2\pi} \langle \tilde{U}_x(q)\,\tilde{U}_x(q')\rangle$$

$$= \iint \frac{dq}{2\pi}\frac{dq'}{2\pi} \frac{2\pi\delta(q+q')\,k_BT}{\kappa q^4+\lambda}$$

$$= \frac{k_BT}{2\pi\lambda}\int_{-\infty}^{+\infty} \frac{dq}{\frac{\kappa}{\lambda}q^4+1}$$

Let $Q = \left(\frac{\kappa}{\lambda}\right)^{1/4}\cdot q$. Then

$$\langle U_x^2(0)\rangle = \frac{k_BT}{2\pi}\,\frac{1}{\lambda^{3/4}\cdot\kappa^{1/4}}\int_{-\infty}^{+\infty}\frac{dQ}{1+Q^4}$$

$$= \frac{1}{2\sqrt{2}}\,\frac{k_BT}{\lambda^{3/4}\kappa^{1/4}}$$

So $\underline{A = \frac{1}{2\sqrt{2}}}$,

1.6) $$\langle U_x^2(0)\rangle = R^2 \iff \lambda^{3/4} = \frac{1}{2\sqrt{2}}\,\frac{k_BT}{\kappa^{1/4}\cdot R^2}$$

$$\iff \underline{\lambda = \frac{1}{4}\,\frac{k_BT^{4/3}}{\kappa^{1/3}\,R^{8/3}}},$$

1.7) For $q \gg q_e = \left(\frac{\lambda}{\kappa}\right)^{1/4}$, the energy is dominated by the <u>bending energy</u> term: the oscillations of the filament are too small for it to see the wall.

For $q \ll q_e$ the energy is dominated by the confinement potential: large-scale oscillations are cheap bending-wise, and <u>bumping into the wall becomes the most predominant penalty</u>.

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1.8) Therefore if L_e is the distance over which bumps into the wall happen we have

$$L_e \approx q_e^{-1} \approx \frac{\kappa^{1/4}}{\lambda^{1/4}}$$

$$\approx \left(\frac{\kappa^{4/3} R^{8/3}}{k_B T^{4/3}}\right)^{1/4}$$

$$\underline{L_e \approx \ell_p^{1/3} R^{2/3}}$$

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II) Linear elastic response

2.1) We have

$$\varphi(0) = \iint \frac{dq}{2\pi}\frac{dq'}{2\pi}\, qq' \langle \tilde{U}_x(q)\tilde{U}_x(q') + \tilde{U}_y(q)\tilde{U}_y(q')\rangle$$

$$= 2\int \frac{dq}{2\pi}(-q^2)\frac{k_B T}{H(q)+\sigma q^2}$$

$$= -2k_B T\int \frac{dq}{2\pi}\frac{q^2}{H(q)}\left(1-\frac{\sigma q^2}{H(q)}\right)$$

$$= \varphi(0) + 2\sigma \cdot k_B T\int_{-\infty}^{+\infty}\frac{dq}{2\pi}\frac{q^4}{H^2(q)}$$

Thus $\varepsilon = k_B T \int_{-\infty}^{+\infty}\frac{dq}{2\pi}\frac{q^4}{H^2(q)}\cdot\sigma$

and thus $\underline{k = \left[k_B T\int_{-\infty}^{+\infty}\frac{q^4}{H^2(q)}\frac{dq}{2\pi}\right]^{-1}}$

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2.2) New length:

$$(\|\vec{R}+\delta\vec{R}\|^2)^{1/2} = \left(\vec{R}^2 + 2\vec{R}\cdot\delta\vec{R} + \delta\vec{R}^2\right)^{1/2}$$

$$\simeq \|\vec{R}^2\|\cdot\left(1+2\frac{\vec{R}\cdot\delta\vec{R}}{\|\vec{R}\|^2}\right)^{1/2}$$

$$\underline{\simeq \|\vec{R}^2\|\cdot\left(1+\frac{\vec{R}\cdot\delta\vec{R}}{\|\vec{R}\|^2}\right)}$$

0.5

So $\varepsilon = \frac{\|\vec{R}+\delta\vec{R}\|}{\|\vec{R}\|} - 1 = \frac{\vec{R}\cdot\delta\vec{R}}{\|\vec{R}\|^2}$

We have $\delta \vec{R} = \tau \cdot \vec{R}$, so

$$\underline{\varepsilon \simeq \frac{\vec{R}^T \cdot \tau \cdot \vec{R}}{\|\vec{R}\|^2} \simeq \hat{R}^T \cdot \tau \cdot \hat{R}}_{0.5}$$

2.3) In spherical coordinates $\hat{R} = \begin{pmatrix} \cos\varphi \sin\theta \\ \sin\varphi \sin\theta \\ \cos\theta \end{pmatrix}$, thus

$$\varepsilon = \begin{pmatrix} \cos\varphi \sin\theta \\ \sin\varphi \sin\theta \\ \cos\theta \end{pmatrix} \cdot \begin{pmatrix} \eta\cos\theta \\ 0 \\ 0 \end{pmatrix} = \eta \cos\theta \sin\theta \cos\varphi$$

So $$E = \frac{k\ell\eta^2}{2} \int_0^{2\pi} \cos^2\varphi \frac{d\varphi}{2\pi} \cdot \int_0^{\pi} \cos^2\theta \sin^3\theta \, d\theta$$

$$= \frac{k\ell\eta^2}{4} \int_0^{\pi} \cos^2\theta \left(1-\cos^2\theta\right) \sin\theta \, d\theta$$

Let $a = \cos\theta$; then

$$E = \frac{k\ell\eta^2}{4} \int_{-1}^{1} a^2(1-a^2)\, da$$

$$= \frac{k\ell\eta^2}{4} \left\{ \left[\frac{a^3}{3}\right]_{-1}^{1} - \left[\frac{a^5}{5}\right]_{-1}^{1} \right\}$$

$$= \frac{k\ell\eta^2}{2} \left(\frac{1}{3} - \frac{1}{5} \right)$$

$$E = \frac{k\ell\eta^2}{15} \quad \text{so } \underline{B = \frac{1}{15}}_{1}$$

2.4) K is the <u>bulk modulus</u>$_{0.5}$. It describes the energetic cost of <u>isotropic deformations</u>$_{0.5}$ of the medium.

2.5) $\gamma_{ij} = \begin{pmatrix} 0 & 0 & \eta/2 \\ 0 & 0 & 0 \\ \eta/2 & 0 & 0 \end{pmatrix}$; thus $\gamma_{kk} = 0$ and

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$$E = \mu \gamma_{ij}\gamma_{ij} = \mu\left[\gamma_{xz}^2 + \gamma_{zx}^2\right]$$

$$\underline{E = \frac{\mu}{2}\eta^2}_{\ 0.5}$$

Therefore $\underline{\mu = \frac{2 k_f}{15}}_{\ 0.5}$

III) <u>Self-consistent determination of the shear modulus</u>

3.1)
$$f_i = -\partial_j \sigma_{ij}$$
$$= -2\mu\,\partial_j\gamma_{ij} + \frac{2\mu}{3}\partial_i \gamma_{kk}$$
$$= -\mu\left(\partial_i\partial_j u_j + \partial_j^2 u_i\right) + \frac{2\mu}{3}\partial_i(\vec{\nabla}\cdot\vec{u})$$
$$= -\mu\,\Delta u_i - \frac{\mu}{3}\partial_i(\vec{\nabla}\cdot\vec{u})$$

Thus

$$\boxed{\begin{aligned} f_x &= -\mu\,\Delta u_x - \frac{\mu}{3}\partial_x(\vec{\nabla}\cdot\vec{u})\\ f_y &= -\mu\,\Delta u_y - \frac{\mu}{3}\partial_y(\vec{\nabla}\cdot\vec{u})\\ f_z &= -\mu\,\Delta u_z - \frac{\mu}{3}\partial_z(\vec{\nabla}\cdot\vec{u})\end{aligned}}_{\ 1}$$

3.2)
$$\tilde{f}_x = \mu k^2 \tilde{u}_x + \frac{\mu}{3} k_x(\vec{k}\cdot\vec{\tilde{u}})$$
$$\tilde{f}_y = \mu k^2 \tilde{u}_y + \frac{\mu}{3} k_y(\vec{k}\cdot\vec{\tilde{u}})$$
$$\tilde{f}_z = \mu k^2 \tilde{u}_z + \frac{\mu}{3} k_z(\vec{k}\cdot\vec{\tilde{u}})$$

We sum

$$k_x\tilde{f}_x + k_y\tilde{f}_y + k_z\tilde{f}_z = \vec{k}\cdot\vec{\tilde{f}}$$
$$= \mu k^2\, \vec{k}\cdot\vec{\tilde{u}} + \frac{\mu}{3}k^2(\vec{k}\cdot\vec{\tilde{u}})$$
$$\vec{k}\cdot\vec{\tilde{f}} = \frac{4\mu}{3}k^2(\vec{k}\cdot\vec{\tilde{u}})$$

Thus $\frac{\mu}{3}\vec{k}\cdot\tilde{\vec{u}} = \frac{\vec{k}\cdot\tilde{\vec{f}}}{4k^2}$

Inserting into the set of three equations:

$$\tilde{f}_i = \mu k^2 \tilde{u}_i + \frac{k_i}{4}\frac{\vec{k}\cdot\tilde{\vec{f}}}{k^2}$$

$$\Rightarrow \quad \mu\tilde{u}_i = \frac{\tilde{f}_i}{k^2} - \frac{1}{4}\frac{\vec{k}\cdot\tilde{\vec{f}}}{k^4}\cdot k_i$$

Thus $\underline{C = \frac{1}{4}}$

3.3) We first compute

$$\tilde{\vec{f}}(\vec{k}) = f_0\hat{x}\cdot\int_{-\infty}^{+\infty}\cos(qz)\,e^{-ik_z z}\,dz \cdot\int_{-\infty}^{+\infty}dx\, e^{-ik_x\cdot x}\,\frac{e^{-\frac{x^2}{2l_i^2}}}{\sqrt{2\pi l_i^2}} \cdot\int_{-\infty}^{+\infty}dy\, e^{-ik_y\cdot y}\,\frac{e^{-\frac{y^2}{2l_i^2}}}{\sqrt{2\pi l_i^2}}$$

$$\underline{\tilde{\vec{f}}(\vec{k}) = f_0\hat{x}\cdot\pi\left[\delta(k_z-q)+\delta(k_z+q)\right]\cdot e^{-\frac{k_x^2+k_y^2}{2}l_i^2}}$$

3.4) $\tilde{\vec{U}}(q) = \int_{-\infty}^{+\infty} dz\,\vec{u}(0,0,z)\,e^{-iqz}$

$$= \int_{-\infty}^{+\infty}dz\,e^{-iqz}\cdot\iint\frac{d^3k}{(2\pi)^3}\,e^{i(k_x 0+k_y 0+k_z z)}\,\tilde{\vec{u}}(\vec{k})$$

$$= \int_{-\infty}^{+\infty}\frac{dk_z}{2\pi}\underbrace{\int_{-\infty}^{+\infty}e^{i(k_z-q)\cdot z}}_{=2\pi\delta(k_z-q)}\cdot\iint\frac{dk_x\,dk_y}{4\pi^2}\,\tilde{\vec{u}}(\vec{k})$$

So $\tilde{\vec{U}}(q) = \iint\frac{dk_x\,dk_y}{4\pi^2}\,\tilde{\vec{u}}(k_x,k_y,q)$

3.4) $\vec{U}(z) = \vec{u}(0,0,z)$

$$= \iint \frac{d^3k}{(2\pi)^3} e^{ik_z \cdot z} \tilde{u}(\vec{k})$$

$$= \frac{1}{\mu} \iint \frac{d^3k}{(2\pi)^3} e^{ik_z \cdot z} \left[\frac{\tilde{f}(\vec{k})}{k^2} - \frac{1}{4} \frac{k_i f_x}{k^4} \vec{k} \right]$$

So the only non-vanishing component of $\vec{U}$ by parity is U_x:

$$U_x(z) = \frac{f_0 \cos(qz)}{4\mu} \cdot \iint \frac{dk_x dk_y}{4\pi^2} e^{-\frac{k_x^2+k_y^2}{2} l_c^2} \left(\frac{4}{q^2+k_x^2+k_y^2} - \frac{k_x^2}{(q^2+k_x^2+k_y^2)^2} \right)$$

$$U_x(z) = \frac{1}{4} \iint \frac{dk_x dk_y}{4\pi^2} \frac{4q^2+4k_y^2+3k_x^2}{(q^2+k_x^2+k_y^2)^2} e^{-\frac{(k_x^2+k_y^2)l_c^2}{2}} \times \frac{f_0 \cos(qz)}{\mu}$$

And thus, defining the 2d vector $\vec{\alpha}$ and scaling $\vec{\alpha} = \vec{k} \cdot l_c$

$$\underline{g^{-1}(\xi) = \iint_{-\infty}^{+\infty} \frac{d^2\alpha}{(2\pi)^2} \frac{\xi^2 + \alpha_y^2 + \frac{3}{4}\alpha_x^2}{(\xi^2+\alpha^2)^2} e^{-\frac{\alpha^2}{2}}}$$

3.5) In Sec. 1, λ is the proportionality coefficient between the displacement of the polymer and the restoring force per unit length. Integrating $\vec{f}(\vec{r})$ over x and y, we find that the force per unit length exerted by the polymer in this section is $f_0 \cos(qz)$. Therefore in Eq. (19) the product μg plays the exact same role as λ. Thus

$$\lambda(q) = \mu g(q l_c)$$

3.6) In Eq. (20):

$$\underline{\mu} \approx \rho k_B T \frac{1}{L_e} \approx \frac{k_B T}{R^2 l_p^{1/3} R^{2/3}} \approx \underline{\frac{k_B T}{R^{8/3} l_p^{1/3}}}$$ 0.5

where we have used $\rho \propto R^{-2}$ and $L_e \approx l_p^{1/3} R^{2/3}$ and the fact that the integral is dominated by $q \approx q_e \approx \frac{1}{L_e}$.
Equation (11) yields

$$\underline{\mu} \approx \rho k \approx \frac{\rho}{k_B T \int \frac{q^4 dq}{(\kappa q^4 + \lambda)^2}} \approx \frac{\rho (k_B T)^2 l_p^2 L_e^5}{k_B T L_e^8}$$

$$\approx \frac{\rho k_B T l_p^2}{L_e^3} \approx \frac{k_B T l_p^2}{R^2 l_p R^2} \approx \underline{k_B T \cdot \frac{l_p}{R^4}}$$ 0.5

3.7) Thus the expression derived under the assumption of affine deformation is larger than the one of Eq. (20) by a factor of 0.5 $\left(\frac{l_p}{R}\right)^{4/3} \gg 1$.

Therefore the system has two geometrically different ways available to it to deform under an externally imposed strain: one is cheap (and non-affine), and the other expensive (and affine). The system will thus choose the cheap option as it wants to minimize its energy. 0.5 Thus we must consider Eq. (20).

3.8) $$1 = \frac{7}{5} \cdot \frac{\rho k_B T}{\mu} \int_{-\infty}^{+\infty} \frac{\mu g(q L_e)}{\kappa q^4 + \mu g(q L_e)} \frac{dq}{2\pi},$$

where we have used Eq. (20) and the result of (3.5).
Letting $\xi = q L_e$:

$$1 = \frac{7}{5} \frac{\rho k_B T}{\mu L_e} \cdot \int_{-\infty}^{+\infty} \frac{\tilde{\mu} g(\xi)}{\xi^4 + \tilde{\mu} g(\xi)} \frac{d\xi}{2\pi}$$

And since $\rho = D R^{-2}$ and $R^2 l_p \propto L_e^3$, we have $\ell = \tilde{D}\,\frac{\ell_p}{L_\xi^3}$ with $\tilde{D}$ a numerical coefficient. Therefore

$$1 = \frac{7\tilde{D}}{5} \cdot \int_{-\infty}^{+\infty} \frac{g(\xi)}{\xi^4 + \tilde{\mu}\, g(\xi)}\, \frac{d\xi}{2\pi},$$

0.5

which constitutes an equation without parameters for $\tilde{\mu}$. The solution must be of the form

$$\tilde{\mu} = \text{a number}$$

$$\Rightarrow \quad \mu \propto \frac{\kappa}{L_\ell^4} \propto \frac{k_B T \ell_p}{\ell_p^{4/3} R^{8/3}} \propto \frac{k_B T}{\ell_p^{1/3} R^{8/3}}$$

0.5