UNIVERSITY OF CAMBRIDGE

MATHEMATICAL TRIPOS Part III

Friday, 18 June, 2021 12:00 pm to 3:00 pm

PAPER 344

THEORETICAL PHYSICS OF SOFT CONDENSED MATTER

Before you begin please read these instructions carefully

Candidates have THREE HOURS to complete the written examination.

*Attempt no more than **THREE** questions.*
*There are **FOUR** questions in total.*
The questions carry equal weight.

STATIONERY REQUIREMENTS
Cover sheet
Treasury tag
Script paper
Rough paper

SPECIAL REQUIREMENTS
None

You may not start to read the questions printed on the subsequent pages until instructed to do so by the Invigilator.

1 *Answer all parts of the question.*

(a) For a system with a conserved scalar order parameter ϕ describing a local composition variable, in which $\mathbb{F} = f(\phi) + \frac{\kappa}{2}(\nabla\phi)^2$, show that minimizing the free energy $F[\phi] = \int \mathbb{F}\, d\mathbf{r}$ at fixed global composition requires the chemical potential $\mu(\mathbf{r}) \equiv \delta F/\delta\phi$ to be constant in space.

(b) For the case $f(\phi) = \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4$ with $a < 0$, consider in mean-field theory an interfacial profile that connects two bulk phases at the binodal densities $\phi = \pm\phi_B = \pm(-a/b)^{1/2}$. Let x be a coordinate perpendicular to the interfaces and take ϕ to be a function of x only. Show that the constant value of μ is zero.

(c) Writing $\phi(x) = \phi_B g(u)$ with $u = x/\xi_0$ and $\xi_0^2 = -2\kappa/a$, establish that

$$2g^2 - g^4 + g'^2 = 1.$$

Hence show that the interfacial profile takes the form $\phi(x) = \pm\phi_B \tanh[(x - x_0)/\xi_0]$. What fixes x_0?

(d) Now consider the more general case where $f(\phi)$ is a smooth symmetric function of ϕ with minima at $\pm\phi_B$, a maximum at $\phi = 0$ and no other turning points; and where $\kappa = \kappa(\phi)$ is any smooth positive function. Give an explicit expression for $\mu(\mathbf{r})$ in terms of ϕ and its spatial derivatives, and show that once again $\mu = 0$ everywhere.

(e) By considering the integral $\int_{\mathcal{V}} \mu(\mathbf{r})\nabla\phi(\mathbf{r})\, d\mathbf{r}$, for an arbitrary domain $\mathcal{V}$, or otherwise, show that in mean-field theory the order parameter $\phi(\mathbf{r})$ in general obeys

$$f(\phi) - \frac{\kappa(\phi)}{2}(\nabla\phi)^2 = \text{constant.}$$

Find the constant, and hence obtain the following equation for (the inverse $x(\phi)$) of the interfacial profile $\phi(x)$:

$$x(\phi) - x_0 = \pm \int_0^{\phi} \sqrt{\frac{\kappa(\psi)}{2(f(\psi) - f(\phi_B))}}\, d\psi. \tag{1}$$

where x_0 is the midpoint position of the profile.

(f) Show also that the interfacial tension obeys

$$\sigma = \int_{-\infty}^{\infty} \kappa(\phi)(\partial_x\phi)^2\, dx.$$

(g) Confirm that for the case in part (c), the solution given for $\phi(x)$ solves Eq.(1).

2 *Answer all parts of the question.*

(a) A certain polar liquid crystal has free energy $F[\mathbf{p}] = \int \mathbb{F}\, d\mathbf{r}$ with

$$\mathbb{F}(\mathbf{p}) = \frac{a}{2}|\mathbf{p}|^2 + \frac{b}{4}|\mathbf{p}|^4 + \frac{\kappa}{2}(\nabla_i p_j)(\nabla_i p_j) \tag{1}$$

where b and κ are positive constants. Explain why for $a < 0$ the equilibrium state consists of uniform $\mathbf{p}$ with magnitude $p_0 = (-a/b)^{1/2}$. Why is this state not reached easily if the system is quenched suddenly from positive to negative a?

(b) Restricting attention to the two dimensional case, briefly explain the concept of topological defects in polar liquid crystals and define the topological charge q. (A detailed exposition of homotopy theory is not required.)

(c) Sketch two different field configurations as examples of $q = +1$ defects and one for a $q = -1$ defect. For the cases with $q = +1$ explain why these two field configurations are topologically equivalent.

(d) Consider in 2D a field configuration $\mathbf{p}(\mathbf{r}) = -p(r)\hat{\mathbf{r}}$. Where is the topological defect and what is its charge? Show that the local free energy density can be written

$$\mathbb{F} = \frac{a}{2}p^2 + \frac{b}{4}p^4 + \frac{\kappa}{2}\left[\left(\frac{dp}{dr}\right)^2 + \left(\frac{p}{r}\right)^2\right].$$

(e) Assuming that p differs from p_0 only in a defect-core region, establish that the resulting F contains an elastic term scaling as $\ln(L/r_0)$ whose coefficient you should calculate. Here L is either the system size or the distance to a neighbouring defect of opposite sign, and r_0 is the size of the core.

(f) State, without detailed calculation, why defects generically dissociate into those of the smallest allowed $|q|$. Briefly explain why for a nematic liquid crystal in 2D, this quantum of charge corresponds to $q = \pm 1/2$ rather than $q = \pm 1$ for the polar case.

(g) Another 2D liquid crystal, comprising a mixture of polar and apolar rodlike molecules, is capable of supporting nematic and polar order simultaneously. Its free energy density is $\mathbb{F} = \mathbb{F}_p + \mathbb{F}_Q + \mathbb{F}_c$ where $\mathbb{F}_p$ obeys Eq.(1) above, $\mathbb{F}_Q = \alpha Q_{ij}Q_{ji} + \beta(Q_{ij}Q_{ji})^2 + K(\nabla_i Q_{ij})(\nabla_k Q_{kj})/2$, and the coupling term is

$$\mathbb{F}_c = -\zeta p_i Q_{ij} p_j/2$$

with β, κ and ζ positive constants. Show that if a and α are chosen negative enough to cause polar and nematic ordering simultaneously, then in any uniform state for which $Q_{ij} = 2\lambda(\hat{n}_i\hat{n}_j - \delta_{ij}/2)$ with $\lambda > 0$, and $\mathbf{p} = p\hat{\mathbf{p}}$, equilibrium requires $\hat{\mathbf{p}} = \pm\hat{\mathbf{n}}$ and $p^2 = -(a - \zeta\lambda)/b$.

(h) Discuss briefly whether half-integer defects can arise in this mixed material.

3 *Answer all parts of the question.*

Consider a one-dimensional manifold in a two-dimensional Euclidean space, parametrised in terms of Cartesian coordinates

$$\mathbf{r}(u) = [x(u), y(u)] \qquad 0 \leqslant u \leqslant 1.$$

(a) (i) Show that the metric

$$g = \frac{\partial \mathbf{r}}{\partial u} \cdot \frac{\partial \mathbf{r}}{\partial u}$$

and the arc-length

$$S(u) = \int_0^u \sqrt{g(u')}\, du'$$

are invariant under the group of isometries $\mathbf{r} \to \mathbf{a} + \mathrm{R}\mathbf{r}$ where $\mathbf{a}$ is a constant vector and R is a constant orthogonal matrix.

(ii) Express the Frenet-Serret equations for the tangent vector

$$\mathbf{t} = \frac{\partial \mathbf{r}}{\partial s} = \frac{1}{\sqrt{g}} \frac{\partial \mathbf{r}}{\partial u}$$

and the unit normal $\mathbf{n}$ as a matrix equation. Explain why this matrix must be antisymmetric.

(iii) Show that the non-zero element of the matrix (i.e. the curvature) is invariant under isometries.

(b) Now consider a moving manifold, a diffeomorphism parametrised by time $t > 0$,

$$\mathbf{r} = \mathbf{r}(u, t)$$

with a velocity $\partial_t \mathbf{r}$. Resolve the velocity in the local frame as

$$\partial_t \mathbf{r}(u, t) = U\mathbf{n} + W\mathbf{t}.$$

(i) Show that compatibility with the Frenet-Serret equations implies for the temporal rates of change, at constant u, of the frame

$$\partial_t \begin{pmatrix} \mathbf{t} \\ \mathbf{n} \end{pmatrix} = \begin{pmatrix} 0 & \partial_s U + kW \\ -\partial_s U - kW & 0 \end{pmatrix} \begin{pmatrix} \mathbf{t} \\ \mathbf{n} \end{pmatrix}$$

and of the invariants

$$\partial_t g = 2g(\partial_s W - kU)$$
$$\partial_t k = (\partial_s^2 + k^2)U + \partial_s k W\,.$$

[QUESTION CONTINUES ON THE NEXT PAGE]

(ii) Hence find an expression for the temporal rate of change of the arc-length.

(c) Assume the one-dimensional manifold is the centerline of a slender rod and is inextensible, i.e. $\partial_t g = 0$.

(i) Write down the equations for the balance of cross-sectional forces $\mathbf{F}$ and moments $\mathbf{M}$ in the presence of forces $\mathbf{f}$ and moments $\mathbf{m}$ per unit length.

(ii) Consider a force per unit length arising from fluid friction and activity

$$\mathbf{f} = -\boldsymbol{\gamma} \cdot \partial_t \mathbf{r} + \mathbf{F}^{\mathrm{A}}$$

where $\boldsymbol{\gamma}$ is a constant friction tensor and show that force balance implies

$$W = \mathbf{t} \cdot \boldsymbol{\mu}(\partial_s \mathbf{F} + \mathbf{f}^{\mathrm{A}})$$
$$U = \mathbf{n} \cdot \boldsymbol{\mu}(\partial_s \mathbf{F} + \mathbf{f}^{\mathrm{A}})$$

where $\boldsymbol{\mu}$ is the inverse of the friction tensor $\boldsymbol{\gamma}$.

(iii) Resolve the force into a tension $F_{\|}$ and a perpendicular force $F_{\perp}$, $\mathbf{F} = F_{\|}\mathbf{t} + F_{\perp}\mathbf{n}$, and likewise $\boldsymbol{\mu} = \mu_{\|}\mathbf{tt} + \mu_{\perp}\mathbf{nn}$, to obtain the invariant forms of the velocities

$$W = \mu_{\|}(\partial_s F_{\|} - kF_{\perp} + f_{\|}^{\mathrm{A}})$$
$$U = \mu_{\perp}(\partial_s F_{\perp} + kF_{\|} + f_{\perp}^{\mathrm{A}})$$

where $\mathbf{f}^{\mathrm{A}} = f_{\|}^{\mathrm{A}}\mathbf{t} + f_{\perp}^{\mathrm{A}}\mathbf{n}$.

4 *Answer all parts of the question.*

(a) A variable $f(t)$ obeys the Langevin equation

$$\dot{f} = -\alpha f + c\Lambda_f(t), \tag{1}$$

where α and c are constants, and $\Lambda_f(t)$ is unit Gaussian white noise such that $\langle\Lambda_f(t)\Lambda_f(t')\rangle = \delta(t-t')$. Confirm the solution $f(t) = c\int_{-\infty}^{t}\Lambda_f(s)e^{-\alpha(t-s)}ds$ and hence, or otherwise, show that

$$\langle f(t)f(t')\rangle = f_0^2 \exp\left(-\alpha|t-t'|\right)$$

with $f_0^2 = c^2/(2\alpha)$.

(b) An overdamped Brownian particle of mobility $\tilde{M}$ moves in a one-dimensional potential V. Its co-ordinate $x(t)$ obeys the Langevin equation

$$\dot{x} = -\tilde{M}V'(x) + (\tilde{M}C^2)^{1/2}\Lambda_x(t)$$

where $\Lambda_x(t)$ is another unit white noise, $V' \equiv dV/dx$, and C is a constant. For a system at equilibrium at temperature T, what should be the value of C? Explain your answer.

(c) A simple model of self-propulsion in one dimension consists of a Brownian particle with $\tilde{M} = 1$ and $V = 0$, and an additional driving force f:

$$\dot{x} = f(t) + C\Lambda_x(t). \tag{2}$$

The driving force f obeys Eq.(1), and there is no correlation between Λ_f and Λ_x. Find $R(t,t') = \langle(x(t)-x(t'))^2\rangle$ and comment on its limiting behaviour for large time intervals, $|t-t'| \gg 1$. You may use without proof the result

$$\int_0^y \int_0^y e^{-|s-s'|}\,ds\,ds' = 2\left(y-1+e^{-y}\right).$$

(d) Now consider a particle in a smooth potential V, with self-propulsion:

$$\dot{x} = -V'(x) + f(t) + C\Lambda_x(t). \tag{3}$$

Let $\mathbb{P}_F[f,x]$ be the probability density for the trajectory $[f(t),x(t)]$, and similarly $\mathbb{P}_B[f,x]$ for the corresponding time-reversed trajectory. For a time-interval $(0,\mathcal{T})$, show that

$$\log\frac{\mathbb{P}_F[f,x]}{\mathbb{P}_B[f,x]} = \Delta U[f,x] + \frac{2}{C^2}\int_0^{\mathcal{T}} \dot{x}(t)f(x(t))\,dt \tag{4}$$

where $\Delta U[f,x]$ is a quantity that you will specify. (It may help to note that, by the usual law of conditional probabilities, $\mathbb{P}[f,x] = \mathbb{P}[f]\,\mathbb{P}[x|f]$.)

(e) Assume that V is everywhere positive. Give the physical interpretation of the three terms that appear in Eq.(4). How do their average values behave for large $\mathcal{T}$? Without additional derivation, describe the expected qualitative behaviour of their probability distributions, at large $\mathcal{T}$.

END OF PAPER