MAMA/344, NST3AS/344, MAAS/344

MAT3 MATHEMATICAL TRIPOS Part III

Friday 31 May 2024 $1:\!30~\mathrm{pm}$ to 3:30 pm

PAPER 344

THEORETICAL PHYSICS OF SOFT CONDENSED MATTER

Before you begin please read these instructions carefully

Candidates have TWO HOURS to complete the written examination.

Attempt no more than **TWO** questions. There are **THREE** 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 A certain system in three dimensions has a conserved scalar order parameter ϕ representing a composition field obeying $\bar{\phi} \equiv \int \phi d\mathbf{r} = 0$. The free energy functional is $F[\phi] = \int \mathbb{F} d\mathbf{r}$ with $\mathbb{F} = f(\phi) + \frac{\kappa}{2} (\nabla \phi)^2 + \frac{\gamma}{2} (\nabla^2 \phi)^2$, where $f = \frac{a}{2} \phi^2 + g |\phi|^3$. Here $\kappa < 0$ and $g, \gamma > 0$. (You are advised to note that the $|\phi|^3$ term is even in ϕ and therefore, not a cubic term in the sense used during the course.)

(a) By neglecting the g term to create a Gaussian model, show that $S(q) \equiv \langle |\phi_{\mathbf{q}}|^2 \rangle = G(q)^{-1}$, assuming this quantity remains positive, where \mathbf{q} is the usual Fourier variable and an explicit expression for G(q) should be given. Show that at this level, as a is reduced, fluctuations first diverge at wavevectors of modulus $q = q_0 = (-\kappa/2\gamma)^{1/2}$. Find a_c , the corresponding critical value of a.

(b) Restoring the g term, evaluate F for a smectic state $\phi(\mathbf{r}) = A \cos q_0 z$ with z an arbitrary axis. You may use without proof that $\int_0^{2\pi} |\cos(u)|^3 du = 8/3$. Show that this gives a continuous transition from isotropic to smectic in which A increases linearly from zero as a falls below a_c .

(c) A variational upper bound \tilde{F} on $F[\phi]$ follows from the inequality

$$F \leqslant \tilde{F} \equiv F_0 - \langle H_0 \rangle + \langle H \rangle_0.$$

Without proving this result, state what is meant by F_0, H_0, H and the notation $\langle \cdot \rangle_0$.

(d) Working within the isotropic phase, show in outline that such an upper bound is

$$\tilde{F} = \sum_{\mathbf{q}}^{+} \left(\ln(J(q)/\pi) - 1 + G(q)/J(q) \right) + g \int \langle |\phi(\mathbf{r})|^3 \rangle_0 \, d\mathbf{r} \tag{*}$$

where J(q) is the kernel of a trial Gaussian model and where the ⁺ superscript on the first term should be defined. Note that you are *not* asked to express the final term in terms of the Fourier amplitudes $\phi_{\mathbf{q}}$ (and are advised not to attempt this!).

(e) Noting that for any Gaussian model $\phi(\mathbf{r})$ is a real Gaussian variable of mean $\bar{\phi} = 0$, show using Parseval's theorem that in d dimensions its variance obeys

$$\langle |\phi(\mathbf{r})|^2 \rangle_0 \equiv \sigma^2 = \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{J(q)} = \frac{1}{(2\pi)^d} \int \frac{d^d \mathbf{r}}{J(q)}$$

where the last equality holds in the large V limit. Using without proof the result that for a real Gaussian variable x of mean zero and variance σ^2 , $\langle |x|^3 \rangle = 4\sigma^3/\sqrt{2\pi}$, find the final term in (*) in terms of J(q).

(f) Construct the best Gaussian approximant to the full theory by minimizing the resulting \tilde{F} with respect to J(q), and show that the latter obeys $J(q) = G(q) + \Delta$ where Δ does not depend on wavevector. Give an explicit expression for Δ in terms of J(q).

(g) Show that this theory predicts a discontinuous transition from the isotropic to the smectic phase for small positive g. Here you can assume without proof that the integral

$$\int \frac{d^d \mathbf{q}}{\bar{a} + \kappa q^2 + \gamma q^4}$$

diverges like $(\bar{a} - a_c)^{-1/2}$ in the limit $\bar{a} \to a_c^+$, where a_c is as defined in part (a) above.

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2 For an isothermal, incompressible binary fluid mixture, the hydrodynamic-level equations read

$$\begin{aligned} (\partial_t + \mathbf{v} \cdot \nabla)\phi &= -\nabla \cdot \mathbf{J} \\ \mathbf{J} &= -M\nabla\mu \\ \rho(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{v} &= \eta\nabla^2 \mathbf{v} - \nabla P - \phi\nabla\mu \\ \nabla \cdot \mathbf{v} &= 0 \\ \mu &= a\phi + b\phi^3 - \kappa\nabla^2\phi \end{aligned}$$

(a) Without deriving these equations, briefly explain why they have this form. Include a statement of what are the order parameters in this system.

(b) In the late stage coarsening of a bicontinuous fluid mixture in three dimensions it is argued that for scaling purposes the time evolution of the characteristic domain size L(t) can be schematically written using the third equation above as

$$\rho(\alpha \ddot{L} + \beta \dot{L}^2/L) = \eta \gamma \dot{L}/L^2 + \sigma \delta/L^2 \tag{(*)}$$

with $\sigma(a, b, \kappa)$ the interfacial tension between phases, and $\alpha, \beta, \gamma, \delta$ dimensionless quantities of order unity. What are the assumptions leading to (*)? Be sure to include a discussion of the pressure term.

(c) Noting that the only combinations of parameters ρ, σ, η with units of length and time are respectively $L_0 = \eta^2 / \rho \sigma$ and $t_0 = \eta^3 / \rho \sigma^2$, find a schematic nondimensionalized version of (*) satisfied by the function f(u) defined via $L(t)/L_0 = f(t/t_0)$.

(d) Find power-law scalings for f(u) such that L(t) becomes independent of (i) ρ and (ii) η , and show that the respective 'viscous hydrodynamic' and 'inertial hydrodynamic' scalings capture the primary balance of terms in (*) at (i) small u and (ii) large u respectively. Show that the crossover time t_X between these regimes is proportional to t_0 .

(e) An experimentalist studies the coarsening problem for a binary fluid placed in a stirring device. This device imposes an additional flow whose root-mean-square velocity gradient is the inverse of a characteristic time τ . The experimentalist reports that the system coarsens until it reaches a steady state domain size $\Lambda(\tau) = g(\tau/t_0)L_0$. Assuming that an algebraic equation for $\Lambda(\tau)$ can be found by the replacement $d/dt \to 1/\tau$ in (*), find a schematic nondimensionalized equation for g(w). Identify regimes of w for which Λ becomes independent of (i) ρ and (ii) η .

(f) State a condition on τ such that inertia dominates over viscosity, and write a brief explanation for the experimentalist saying why this regime corresponds to low velocity gradients rather than high ones. (The experimentalist worries that in all fluid-mechanical problems they have previously worked on, the opposite is true.)

3 A system is described by a coarse-grained vector order parameter field $\mathbf{p}(\mathbf{r}, t)$ which obeys the Langevin equation

$$\dot{\mathbf{p}}(\mathbf{r},t) = -\Gamma \frac{\delta F}{\delta \mathbf{p}(\mathbf{r},t)} + \mathbf{f}(\mathbf{r},t) \tag{\dagger}$$

where $F[\mathbf{p}(\mathbf{r})]$ is the free energy, Γ a constant coefficient, and \mathbf{f} is Gaussian white noise of probability density $\mathbb{P}[\mathbf{f}(\mathbf{r},t)] = \mathcal{N} \exp\left[-\frac{1}{2\sigma^2} \int |\mathbf{f}(\mathbf{r},t)|^2 d\mathbf{r} dt\right]$ with \mathcal{N} a normalization constant. The noise is caused by coupling to a heat bath at temperature T.

(a) State the probability density $\mathbb{P}_F[\mathbf{p}(\mathbf{r}, t)]$ for a time evolution $\mathbf{p}(\mathbf{r}, t)$ connecting an initial configuration $\mathbf{p}_1(\mathbf{r}, t_1)$ of free energy F_1 to a final configuration $\mathbf{p}_2(\mathbf{r}, t_2)$ of free energy F_2 . Write down $\mathbb{P}_B[\mathbf{p}(\mathbf{r}, t)]$, the probability density for the time-reversed trajectory. State any assumptions made about the normalization factors involved.

(b) Show that

$$\frac{\mathbb{P}_F}{\mathbb{P}_B} = \exp\left[-\frac{2\Gamma}{\sigma^2}\int_{t_1}^{t_2}dt\int\dot{\mathbf{p}}\frac{\delta F}{\delta\mathbf{p}}\,d\mathbf{r}\right]$$

and explain why, if the underlying microscopic dynamics has time-reversal symmetry, this implies that $\sigma^2 = 2\Gamma k_B T$.

(c) Consider the case where $\delta F/\delta \mathbf{p} = a\mathbf{p} - \kappa \nabla^2 \mathbf{p}$ with $a, \kappa > 0$. Suppose that the system is initially in equilibrium with $a = a_I$ and then at time t_1 , the value of a is suddenly changed to a final value a_F . Confirm that, in Fourier variables, for times $t > t_1$, the amplitudes obey $\mathbf{p}_{\mathbf{q}}(t) = \mathbf{p}_{\mathbf{q}}(t_1) \exp\left[-r(q)(t-t_1)\right] + \int_{t_1}^t \mathbf{f}_{\mathbf{q}}(t') \exp\left[-r(q)(t-t')\right] dt'$ and give an expression for the decay rate r(q).

(d) Hence show the following result for the equal-time correlator $\langle p_{\mathbf{q},i}(t_2)p_{-\mathbf{q},j}(t_2)\rangle$ at times $t_2 > t_1$, where $p_{\mathbf{q},i}$ is the *i*th Cartesian component of the vector $\mathbf{p}_{\mathbf{q}}$:

$$\langle p_{\mathbf{q},i}(t_2)p_{-\mathbf{q},j}(t_2)\rangle = \delta_{ij} \left[\frac{k_B T}{a_I + \kappa q^2} e^{-2r(q)(t_2 - t_1)} + \frac{k_B T}{a_F + \kappa q^2} \left(1 - e^{-2r(q)(t_2 - t_1)} \right) \right].$$

You may assume without proof that the Fourier transform of the noise in (†) obeys $\langle f_{\mathbf{q},i}(t)f_{-\mathbf{q},j}(t')\rangle = 2k_B T \Gamma \delta_{ij} \delta(t-t')$. Briefly interpret the above result.

(e) By generalizing the above calculation, find also the unequal-time correlator $\langle p_{\mathbf{q},i}(t_2)p_{-\mathbf{q},j}(t_3)\rangle$ for all $t_{2,3} > t_1$ and confirm that for $t_2, t_3 \gg t_1$ this approaches

$$\frac{k_B T}{a_F + \kappa q^2} e^{-r(q)|t_3 - t_2|}$$

END OF PAPER

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