

## PROBLEM SET 2

Notes:

- This set contains 2 problems, with multiple parts to each problem.
- Please start each problem on a new page.
- Due date: November 1, 2005.

### 1 Elasticity in two dimensions

Consider the quadratic field theory for displacements in a solid discussed in class in which the probability of observing the Fourier-transform  $\mathbf{u}(\mathbf{k})$  of the displacement field  $\mathbf{u}(\mathbf{x})$  is

$$P(\mathbf{u}(\mathbf{k})) = \frac{e^{-\beta V[\mathbf{u}(\mathbf{k})]}}{\int \mathcal{D}\mathbf{u}(\mathbf{k}) e^{-\beta V[\mathbf{u}(\mathbf{k})]}}$$

with

$$V[\mathbf{u}(\mathbf{k})] = V^* + \int \frac{d\mathbf{k}}{(2\pi)^2} \left[ \frac{\mu}{2} k^2 |\mathbf{u}(\mathbf{k})|^2 + \frac{\mu + \lambda}{2} (\mathbf{k} \cdot \mathbf{u}(\mathbf{k}))^2 \right].$$

- a. Show that the *transverse modes*  $u_t(\mathbf{k})$  with  $\mathbf{k} \perp \mathbf{u}$ , and the *longitudinal modes*, with  $u_l(\mathbf{k}) = \hat{\mathbf{k}} \cdot \mathbf{u}(\mathbf{k})$ , have energies,

$$H_T = \frac{\mu}{2} \int \frac{d\mathbf{k}}{(2\pi)^2} k^2 |u_t(k)|^2$$

$$H_l = \frac{(2\mu + \lambda)}{2} \int \frac{d\mathbf{k}}{(2\pi)^2} k^2 |u_l(k)|^2$$

respectively.

- b. Show that the correlation function of the displacement field  $\mathbf{u}(\mathbf{k})$  is

$$\langle u_i(\mathbf{k}) u_j(\mathbf{k}') \rangle = \frac{(2\pi)^2 kT \delta(\mathbf{k} + \mathbf{k}')}{\mu k^2} \left[ \delta_{ij} - \frac{\mu + \lambda}{2\mu + \lambda} \frac{k_i k_j}{k^2} \right].$$

- c. Show that the extent of fluctuations in real space is given by

$$\langle (\mathbf{u}(\mathbf{x}) - \mathbf{u}(0))^2 \rangle \sim \frac{kT}{\mu} \left( \frac{3\mu + \lambda}{2\mu + \lambda} \right) \frac{\ln(|\mathbf{x}|/a)}{\pi}$$

at large distances  $|\mathbf{x}| \gg a$ , where  $a$  is the lattice spacing. What does this imply about the stability of the ordered phase?

- d. Evaluate the average of fluctuations  $\langle \rho_k(\mathbf{x}) \rho_k^*(0) \rangle$  of the *order parameter*  $\rho_k(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$  for the solid-liquid transition. How does this compare with the result in 3-dimensions?
- e. The crystal phase, taken here to be on a triangular lattice in the  $x - y$  plane, is also characterized by a broken *rotational* symmetry. We can define an *orientational order parameter*,  $\Psi(\mathbf{x}) = e^{6i\theta(\mathbf{x})}$ , where  $\theta(\mathbf{x})$  is the angle between the lattice bonds and a fixed reference axis and the factor of 6 accounts for the equivalence of the 6 possible directions of the triangular lattice. The distortion  $\mathbf{u}(\mathbf{x})$  leads to a change in bond angle given by

$$\theta(\mathbf{x}) = -\frac{1}{2} \left( \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right) = -\frac{1}{2} \hat{\mathbf{z}} \cdot \nabla \times \mathbf{u}.$$

Show that the decay of *orientational fluctuations* is

$$\langle \Psi(\mathbf{x}) \Psi^*(0) \rangle = \langle e^{i6(\theta(\mathbf{x}) - \theta(0))} \rangle \sim \exp \left\{ -\frac{9kT}{\mathbf{a}^2 \mu} \right\}$$

at large distances. Note that this result implies that the two-dimensional solid is characterized by quasi-long-range translational order and true long-range orientational order.

## 2 Density Functional Theory: Freezing of a hard sphere liquid

- a. Show that the difference  $\Delta W$  in the grand potential,  $W = -\Omega = F - \int d\mathbf{r} \bar{\rho}(\mathbf{r}) \psi(\mathbf{r})$ , between the solid and liquid phases at a solid-liquid equilibrium point can be written by expanding to quadratic order in the density difference  $\Delta \bar{\rho}(\mathbf{r}) = \bar{\rho}(\mathbf{r}) - \rho_l$  around the uniform fluid density  $\rho_l$  to obtain

$$\Delta W[\bar{\rho}] = V \rho_l + \int d\mathbf{r} \bar{\rho}(\mathbf{r}) (\ln \bar{\rho}(\mathbf{r}) / \rho_l - 1) - \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \Delta \bar{\rho}(\mathbf{r}) c(|\mathbf{r} - \mathbf{r}'|) \Delta \bar{\rho}(\mathbf{r}'),$$

where  $c(|\mathbf{r} - \mathbf{r}'|)$  is the direct correlation function for the uniform liquid.

- b. Defining  $\omega[\bar{\rho}(\mathbf{r})] = \Delta W[\bar{\rho}(\mathbf{r})] / V \rho_l$ , show that  $\omega$  can be written as

$$\begin{aligned} \omega &= 1 + \frac{\rho_s}{\rho_l} \int_{\Delta} d\mathbf{r} \rho(\mathbf{r}|0) (\ln \rho(\mathbf{r}|0) \rho_l - 1) + \rho_s \hat{\rho}(0) \hat{c}(0) \\ &\quad - \frac{1}{2} \rho_l \hat{c}(0) - \frac{\rho_s^2}{2\rho_l} \sum_{\mathbf{G}} \hat{c}(\mathbf{G}) \hat{\rho}(\mathbf{G})^2, \end{aligned}$$

where  $\Delta$  is the cell volume,  $\rho_s = 1/\Delta$  is the bulk density of the solid,  $\hat{c}(\mathbf{G})$  is the *infinite* space Fourier transform of  $c(r)$ , and  $\mathbf{G}$  are the set of reciprocal lattice vectors. In the equation above, we have used that the Fourier transform and back transform of an arbitrary periodic function  $f$  are defined as

$$\hat{f}(\mathbf{G}) = \int_{\Delta} d\mathbf{r} e^{-i\mathbf{G}\cdot\mathbf{r}} f(\mathbf{r}) \quad f(\mathbf{r}) = \frac{1}{\Delta} \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \hat{f}(\mathbf{G}).$$

c. Following our work on elasticity theory, assume that the unit cell density  $\rho(\mathbf{r} - \mathbf{R}|\mathbf{R}) \sim \exp\{-(\mathbf{r} - \mathbf{R})^2/\epsilon^2\}$  is Gaussian-distributed around the center of the cell located at  $\mathbf{R}$ . Note that we have reduced the expression for  $\omega$  to one involving only the  $\rho(\mathbf{r} - \mathbf{R}|\mathbf{R})$  centered at the origin. Assuming that there is a single particle in each cell and that the Gaussian has decayed to zero before the cell boundary is reached:

- Show that  $\hat{\rho}(\mathbf{G}) = \exp\{-G^2\epsilon^2/4\}$ .
- Verify that

$$\int_{\Delta} d\mathbf{r} \rho(\mathbf{r}|0) (\ln \rho(\mathbf{r}|0)\rho_l - 1) = -\frac{5}{2} - \ln \rho_l - 3 \ln(\sqrt{\pi}\epsilon).$$

- d. For an FCC lattice, find the set of reciprocal lattice vectors  $\mathbf{G}$  such that  $\mathbf{G} \cdot \mathbf{R} = 2\pi k$ , where  $\mathbf{R} = l\mathbf{T}_1 + m\mathbf{T}_2 + n\mathbf{T}_3$  and  $k$  is an integer. (Hint: let  $\mathbf{G} = \tilde{l}\mathbf{b}_1 + \tilde{m}\mathbf{b}_2 + \tilde{n}\mathbf{b}_3$  where  $\mathbf{b}_i \cdot \mathbf{T}_j = 2\pi\delta_{ij}$ .)
- e. Compute the Fourier transform of the direct correlation function  $\hat{c}(G)$  using the Percus-Yevick solution for the direct correlation function:

$$c(r/\sigma) = \begin{cases} b_0 + b_1(r/\sigma) + b_2(r/\sigma)^3 & 0 \leq r/\sigma \leq 1 \\ 0 & 1 < r/\sigma \end{cases}$$

where  $\sigma$  is the diameter of the hard sphere particles and

$$\begin{aligned} b_0 &= -\frac{(1+2\eta)^2}{(1-\eta)^4} & b_1 &= \frac{6\eta(1+\eta/2)^2}{(1-\eta)^4} \\ b_2 &= -\frac{\eta(1+2\eta)^2}{(1-\eta)^4} & \eta &= \pi\rho_l/6. \end{aligned}$$

- f. Using the information from all the parts above, implement a numerical routine to compute the density at which the hard sphere fluid of diameter  $\sigma$  freezes into an FCC solid. You may use any scheme you wish to find either the global minimum of  $\omega$  as a function of the parameters  $\epsilon$  and  $a$ , or a root-search method to find the solution of the minimization equations.