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Physics 704 **HOMEWORK ASSIGNMENT #2** Fall 2011

Study: P&B 5.2, 5.4, 3.6
Skim: P&B 5.1, 5.3, 5.5

Due date for problems on Tuesday, March 1 [deadline on March 3].

1. P&B problem 5.1 Note that these particles are distinguishable. (In your solution , explain why.) In part (a), you should argue first that $Z = [L - N\,a]^N/N!$. In (b) state clearly what form *f* takes for this potential.

2. Show (rather trivially) that a) The Percus-Yevick closure (eq. 5.46) can be rewritten as
$C(r) = g(r) - y(r)$.
and b) The hypernetted chain closure (eqn. 5.48) can be written as
$g(r) = \exp[h(r) - \beta U(r) - C(r)]$.

c) The above two closures (using the form in P&B or from above) are then to be inserted into the Ornstein-Zernike equation to get the Percus-Yevick and hypernetted chain integral equations, respectively. Derive these expressions:

$$g(r_{12})\exp(\beta U(r_{12})) = 1 - n\int d^3r_3\,[\exp(\beta U(r_{23})) - 1]g(r_{23})\,[g(r_{13}) - 1] \quad \text{(PY) and}$$

$$\ln g(r_{12}) = -\beta U(r_{12}) + n\int d^3r_3\,[g(r_{23}) - 1 - \ln g(r_{23}) - \beta U(r_{23})]\,[g(r_{13}) - 1] \quad \text{(HNC)}$$

3. Consider a simple cubic lattice with lattice constant *a* (at T=0). For full symmetry, we can consider a slab that is *n* layers thick, with periodic boundary conditions in the 2 in-plane (x-y) directions. In that plane, the cell need only contain a single atom.
a) Argue that the energy of this construction in an electronic structure calculation is

$$nE_B + 2E_S$$

where E_B is the bulk energy per atomic volume and E_S is the surface energy per atomic area.
b) If another "layer" is added (so another atom), what is the total energy?
c) Use this information to indicate how to separate out E_B and E_S when computing slab energies.

d) Suppose one next seeks to evaluate the energy of an added close-packed step on this surface. Assuming that the surface of the slab is a rectangle of sides L_x and L_y, create a pair of steps by adding a strip of material of width L running across the surface (so that the side view looks like an anti-dado [anti-groove]). Assuming that you know E_B and E_S from previous work and that L is large enough so that the steps do not interact, write and expression for the *step energy per length* γ. Your expression should not require that the riser of the step is perpendicular to the surface (although it is in this example).

Added note: It is clearer if you consider the total energy of a slab to have the form

$$N \varepsilon_0 + 2 \sigma L_x L_y$$

where N is the total number of atoms, ε_0 is the cohesive energy per atom, and σ is the surface energy per area. For simplicity, assume the atoms are unit cubes. (What is the relation between E_B and ε_0?)

4. Problem on capillary waves (i.e. capillary-gravitational waves in the limit that $a^{-1} \to 0$).

a) Show that the capillary waves $\check{z}_{\mathbf{q}}$ are Goldstone modes. [1] To what symmetry breaking are they related?

b) Compute the height-height correlation function $G(\boldsymbol{\rho},\boldsymbol{\rho}') = G(\boldsymbol{\rho}-\boldsymbol{\rho}') = \langle [z(\boldsymbol{\rho})-z(\boldsymbol{\rho}')]^2 \rangle$ in terms of a multiple integral over $\langle (\check{z}_{\mathbf{q}}\ \check{z}_{\mathbf{q}'})^2 \rangle$, where $\boldsymbol{\rho} = (x,y)$.

c) Show that for large separations G behaves as $\ln |\boldsymbol{\rho} - \boldsymbol{\rho}'|$.
(In $d = 2$ and 1 it goes like $|\boldsymbol{\rho} - \boldsymbol{\rho}'|^{3\text{-d}}$.)

~~5. P&B problem 3.8~~ (postponed to Set 3)

[1] A Goldstone mode has an energy that vanishes as $\lambda \to \infty$ (or $q \to 0$). It corresponds to a broken *continuous* symmetry. Rotations from one ordered state to another costs vanishingly little energy. In field theory, such modes are sometimes called "massless." Phonons in solids are the most familiar example, with the crystal structure breaking translational [and rotational] symmetry. See, e.g., Kardar, *Stat. Phys. of Fields*