

## Statistical Physics II

### Problem Set 5

Due: Tuesday, May 13, **before** the lecture

#### 6. Functional derivatives (4 points)

The functional derivative  $\delta F[\phi]/\delta\phi$  of a functional  $F$  of the function  $\phi(\mathbf{r})$  is defined via

$$\left. \frac{d}{d\varepsilon} F[\phi + \varepsilon\eta] \right|_{\varepsilon=0} = \int d^d r \frac{\delta F[\phi(\mathbf{r})]}{\delta\phi(\mathbf{r})} \eta(\mathbf{r}).$$

Calculate the functional derivative with respect to  $\phi(\mathbf{r})$  for the following examples:

- i)  $F[\phi] = \phi(\mathbf{r}')$
- ii)  $F[\phi] = \int d^d r' V(\phi(\mathbf{r}'))$
- iii)  $F[\phi] = \frac{1}{2} \int d^d r' [\nabla\phi(\mathbf{r}')]^2$ .

Choose a suitable test function  $\eta(\mathbf{r})$ , e.g. a  $\delta$ -function. If necessary, use integration by parts, where the variation on the boundary of the volume (at infinity) vanishes.

#### 7. Density functional theory (4 points + 4 additional points)

##### a) *Direct correlation function*

Derive from the definition of the direct correlation function,

$$c(\vec{r}, \vec{r}') = \frac{1}{n(\vec{r})} \delta(\vec{r} - \vec{r}') - \beta \frac{\delta\mu(\vec{r})}{\delta n(\vec{r}')} ,$$

the Ornstein-Zernicke integral equation.

*Hint:* Use  $G(\vec{r}, \vec{r}') = n(\vec{r})h(\vec{r}, \vec{r}')n(\vec{r}') + n(\vec{r})\delta(\vec{r} - \vec{r}')$ , the generalization of the known relation  $g(r) = h(r) + 1$  between the corresponding quantities in homogeneous fluids.

b) *Barometer equation*

Calculate for the boundary condition  $n(0) = n_0$  the chemical potential  $\mu$  and the position-dependent density  $n(\vec{r})$  of an inhomogeneous temperature-controlled ideal gas in the one-particle potential  $\mu(\vec{r}) = \mu - u(\vec{r})$  with  $u(0) = 0$ . Take as a starting point the known density functional for the free energy of an inhomogeneous ideal gas and the minimum condition on the grand-canonical potential.

c\*) *Microphase separation in “random phase approximation” (RPA)*

In the so-called RPA-approximation, the free energy  $F^{(0)}$  of the reference system (containing short range interactions,  $r \simeq \sigma$ ) is expanded on by the term

$$F_{\text{ex}}(\delta(\mathbf{r})) = \frac{1}{2} \int d^3r d^3r' \nu_1(\mathbf{r} - \mathbf{r}') \delta n(\mathbf{r}) \delta n(\mathbf{r}'),$$

where the weak long range pair-potential  $\nu_1$  is considered as a perturbation. For a homogeneous fluid show that  $S_{\mathbf{q}}^{-1} = (S_{\mathbf{q}}^{(0)})^{-1} + n\beta\nu_{1\mathbf{q}}$  holds and that the structure factor, for the perturbation potential

$$\nu_1(r) = u_1 e^{-\kappa_1 r} - u_2 e^{-\kappa_2 r},$$

where  $\kappa_1 < \kappa_2 \ll \sigma^{-1}$ ,  $0 < \beta u_1 < \beta u_2 \ll 1$ , develops a small-angle peak with

$$S_{\mathbf{q} \rightarrow 0}^{-1} \sim a + b(q^2/q_0^2 - 1)^2.$$

Discuss its physical relevance and the contribution of the long range interaction to the isothermal compressibility, as a function of the potential parameters.

**Total score: 8+4 points**