Lecture 6 alt: Gaussian Functional Integrals

Tuesday, June 21, 2022 8:00 AM

From weak inhomogeneity expansion, we've seen that we can write

$$Q[w] \approx e^{-\mu_0}\left[1 - \frac{N^2}{2V^2}\sum_k g_k w_k w_{-k}\right]$$

Using $\log(1-x) \approx -x$ + the above approximation, we can manipulate our effective Hamiltonian to

$$\mathcal{H} \approx \frac{1}{2V}\sum \gamma_k w_k w_{-k}$$

So $\mathcal{H}$ is quadratic in w_k, + our partition fn is:

$$Z = e^{-\beta F} = \frac{z_0}{n!\,\Omega_0}\int \mathcal{D}w\, e^{-\frac{1}{2V}\sum_k \gamma_k w_k w_{-k}}$$

We can show that this is a solvable Gaussian integral

It gives analytic results for F, which allows deriving

μ, P, + finding equilibrium conditions

There are a lot of subtleties to get right... (Villet + GHF, JCP 2014)

1. $\int \mathcal{D}w$ is an integral over the real axis of $w(r)$, despite $e^{-\mathcal{H}}$ being generally complex
   - Think of the analogy to inv. FT: $\int dk$ is real vals of k

2. By adding or subtracting an imaginary constant, we can deform the integrals to be along the real axis

3. For a purely real function $w(r)$, $w(k)$ & $w(-k)$ are complex conjugates of each other

$$w_k = w_k^R + i\,w_k^I \qquad w_{-k} = w_k^R - i\,w_k^I$$

4. Integrating over all forms of a function $\int \mathcal{D}w$ can be done in real space or Fourier space, & we can discretize these integrals in real or Fourier space

$$\int \mathcal{D}w \approx \prod_r^M \int dw_r = \int_{-\infty}^{\infty} dw_0 \prod_{\underline{k}}{}' \int_{-\infty}^{\infty} dw_{\underline{k}}^R \int dw_{\underline{k}}^I = \prod_k{}' \int_{-\infty}^{\infty} dw_k^R \int dw_k^I$$

The $'$ on the sum is to indicate that you must have the same # of integrals in real space & k-space
There's $\sim \frac{1}{2}$ as many over w_k^R as w_r

With all of this in mind, we can solve some integrals

Ω_0 from Model A's partition function:

$$\Omega_0 = \int \mathcal{D}w\, e^{-\frac{1}{2u_0}\int dr\,[w(r)]^2} = \int \mathcal{D}w\, e^{-\frac{1}{2u_0 V}\sum_k w_k w_{-k}}$$

$$\Omega_0 = \int \mathcal{D}w \, e \qquad = \int \mathcal{D}w \, e$$

$$= \prod_k \int_{-\infty}^{\infty} dw_k^R \int_{-\infty}^{\infty} dw_k^I \, e^{-\frac{1}{2u_0 V} \sum_k (w_k^R)^2 + (w_k^I)^2}$$

This is an exponential of a bunch of sums - all the integrals are identical!

$$\Omega_0 = \prod_k \int_{-\infty}^{\infty} dw \, e^{-\frac{1}{2u_0 V} w^2} = \prod_k \sqrt{2\pi V} = (2\pi V)^{M/2}$$

Go back to the Edward's model:

$$Z = \frac{z_0^n}{n! \, \Omega_0} \int \mathcal{D}w \, e^{-\mathcal{H}}$$

$$\mathcal{H} = \frac{1}{2u_0} \int dr \, [w(r)]^2 - n \log Q$$

$$Q = e^{-w_0} \left[1 - \frac{N^2}{2V} \sum_k g_k w_k w_{-k} \right]$$

$$\mathcal{H} = \frac{1}{2u_0 V} \sum_k w_k w_{-k} + n w_0 + \frac{n N^2}{2V^2} \sum_k g_k w_k w_{-k}$$

$$\mathcal{H} = \frac{1}{2V} \sum_k \underbrace{\left(\frac{1}{u_0} + \rho_0 N g_k \right)}_{\gamma_k} w_k w_{-k} \overset{+ n w_0}{=} \frac{1}{2V} \sum_k \gamma_k w_k w_{-k} + n w_0$$

$$Z = \frac{z_1^n}{n! \, \Omega_0} \prod_k \int dw_k^R \int dw_k^I \, e^{-\frac{1}{2V} \sum_k \gamma_k \left[(w_k^R)^2 + (w_k^I)^2 \right]}$$

$$Z = \frac{z_1^n}{n!\,\Omega_0} \prod_k \sqrt{\frac{2\pi V}{\gamma_k}} = e^{-\beta F}$$

$$\beta F = -\log Z = -n \log z_1 + \log n! + \log \Omega_0 + \frac{1}{2}\sum_k \log \frac{\gamma_k}{2\pi V}$$

$$\beta F_{fluct} = \frac{1}{2}\sum_k \log\left(\frac{1}{u_0} + \rho_0 N g_k\right) = \frac{1}{2}\sum_k \log(1 + u_0 \rho_0 N g_k)$$

$\times$ + $\div$ by u_0

$$= \frac{V}{2V}\sum_{\underline{k}} \log(1 + u_0 N \rho_0 g_k) \approx \frac{V}{2}\frac{1}{(2\pi)^3}\int d\underline{k}\, \log(1 + u_0 N \rho_0 g_k)$$

$$= \frac{V}{4\pi^2}\int_0^{\Lambda_c} dk\, k^2 \log(1 + u_0 N \rho_0 g_k)$$

cut-off stops the UV-divergence

Total free energy including mean-field terms:

$$\beta F = F_0 + \frac{1}{2}\rho_0^2 u_0 \cdot V + \frac{V}{4\pi^2}\int_0^{\Lambda_c} dk\, k^2 \log(1 + u_0 N \rho_0 g_k)$$

Can get μ from $\frac{\partial F}{\partial n}$, p from $-\frac{\partial F}{\partial V}$ $\quad \rho_0 = \frac{nN}{V}$