II.G Gaussian Integrals

In the previous section, the energy cost of fluctuations was calculated at quadratic order. These fluctuations also modify the saddle point free energy. Before calculating this modification, we take a short (but necessary) mathematical diversion on performing Gaussian integrals.

The simplest Gaussian integral involves one variable ϕ,

$$\mathcal{I}_1 = \int_{-\infty}^{\infty} d\phi \, e^{-\frac{K}{2}\phi^2 + h\phi} = \sqrt{\frac{2\pi}{K}} \, e^{\frac{h^2}{2K}}. \tag{II.54}$$

By taking derivatives of the above expression with respect to h, integrals involving powers of ϕ are generated; e.g.

$$\begin{aligned} \frac{d}{dh}: &\qquad \int_{-\infty}^{\infty} d\phi \; \phi \, e^{-\frac{K}{2}\phi^2 + h\phi} = \sqrt{\frac{2\pi}{K}} e^{\frac{h^2}{2K}} \cdot \frac{h}{K}, \\ \frac{d^2}{dh^2}: &\qquad \int_{-\infty}^{\infty} d\phi \; \phi^2 e^{-\frac{K}{2}\phi^2 + h\phi} = \sqrt{\frac{2\pi}{K}} e^{\frac{h^2}{2K}} \cdot \left[\frac{1}{K} + \frac{h^2}{K^2}\right]. \end{aligned} \tag{II.55}$$

If the integrand represents the probability density of the random variable ϕ, the above integrals imply the moments $\langle\phi\rangle = h/K$, and $\langle\phi^2\rangle = h^2/K^2 + 1/K$. The corresponding cumulants are $\langle\phi\rangle_c = \langle\phi\rangle = h/K$, and $\langle\phi^2\rangle_c = \langle\phi^2\rangle - \langle\phi\rangle^2 = 1/K$. In fact all higher order cumulants of the Gaussian distribution are zero since

$$\left\langle e^{-ik\phi}\right\rangle \equiv \exp\left[\sum_{\ell=1}^{\infty} \frac{(-ik)^\ell}{\ell!} \left\langle \phi^\ell \right\rangle_c\right] = \exp\left[-ikh - \frac{k^2}{2K}\right]. \tag{II.56}$$

Now consider the following Gaussian integral involving N variables,

$$\mathcal{I}_N = \int_{-\infty}^{\infty} \prod_{i=1}^{N} d\phi_i \exp\left[-\sum_{i,j} \frac{K_{i,j}}{2}\phi_i\phi_j + \sum_i h_i\phi_i\right]. \tag{II.57}$$

It can be reduced to a product of N one dimensional integrals by diagonalizing the matrix $\mathbf{K} \equiv K_{i,j}$. Since we need only consider *symmetric matrices* ($K_{i,j} = K_{j,i}$), the eigenvalues are real, and the eigenvectors can be made orthonormal. Let us denote the eigenvectors and eigenvalues of $\mathbf{K}$ by $\hat{q}$ and K_q respectively, i.e. $\mathbf{K}\hat{q} = K_q\hat{q}$. The vectors $\{\hat{q}\}$ form a new coordinate basis in the original N dimensional space. Any point in this space can be represented either by coordinates $\{\phi_i\}$, or $\left\{\tilde{\phi}_q\right\}$ with $\phi_i = \sum_q \tilde{\phi}_q\hat{q}_i$. We can now change the integration variables from $\{\phi_i\}$ to $\left\{\tilde{\phi}_q\right\}$. The Jacobian associated with this unitary transformation is unity, and

$$\mathcal{I}_N = \prod_{q=1}^{N} \int_{-\infty}^{\infty} d\tilde{\phi}_q \exp\left[-\frac{K_q}{2}\tilde{\phi}_q^2 + \tilde{h}_q\tilde{\phi}_q\right] = \prod_{q=1}^{N} \sqrt{\frac{2\pi}{K_q}} \exp\left[\frac{\tilde{h}_q K_q^{-1} \tilde{h}_q}{2}\right]. \qquad \text{(II.58)}$$

The final expression can be represented in terms of the original coordinates by using the *inverse* matrix $\mathbf{K^{-1}}$, such that $\mathbf{K^{-1}K} = \mathbf{1}$. Since the determinant of the matrix is independent of the choice of basis, $\det \mathbf{K} = \prod_q K_q$, and

$$\mathcal{I}_N = \sqrt{\frac{(2\pi)^N}{\det \mathbf{K}}} \exp\left[\sum_{i,j} \frac{K_{i,j}^{-1}}{2} h_i h_j\right]. \qquad \text{(II.59)}$$

Regarding $\{\phi_i\}$ as Gaussian random variable distributed with a joint probability distribution function proportional to the integrand of eq.(II.57), the *joint characteristic function* is given by

$$\left\langle e^{-i\sum_j k_j\phi_j} \right\rangle = \exp\left[-i\sum_{i,j} K_{i,j}^{-1} h_i k_j - \sum_{i,j} \frac{K_{i,j}^{-1}}{2} k_i k_j\right]. \qquad \text{(II.60)}$$

Moments of the distribution are obtained from derivatives of the characteristic function with respect to k_i, and *cumulants* from derivatives of its logarithm. Hence, eq.(II.60) implies

$$\begin{cases} \langle \phi_i \rangle_c = \sum_j K_{i,j}^{-1} h_j \\ \langle \phi_i \phi_j \rangle_c = K_{i,j}^{-1} \end{cases}. \qquad \text{(II.61)}$$

Another useful form of eq.(II.60) is

$$\langle \exp(A) \rangle = \exp\left[\langle A \rangle_c + \frac{1}{2}\langle A^2 \rangle_c\right], \qquad \text{(II.62)}$$

where $A = \sum_i a_i \phi_i$ is any linear combination of Gaussian distributed variables. We used this result earlier in computing the order parameter correlations in the presence of phase fluctuations in a superfluid.

Gaussian *functional integrals* are a limiting case of the above many variable integrals. Consider the points i as the sites of a d–dimensional lattice and let the spacing go to zero.

In the continuum limit, $\{\phi_i\}$ go over to a function $\phi(\mathbf{x})$, and the matrix K_{ij} is replaced by a *kernel* $K(\mathbf{x},\mathbf{x}')$. The natural generalization of eq.(II.59) is

$$\begin{aligned}&\int_{-\infty}^{\infty}\mathcal{D}\phi(\mathbf{x})\exp\left[-\int d^d\mathbf{x}d^d\mathbf{x}'\frac{K(\mathbf{x},\mathbf{x}')}{2}\phi(\mathbf{x})\phi(\mathbf{x}')+\int d^d\mathbf{x}h(\mathbf{x})\phi(\mathbf{x})\right]\\&\propto(\det\mathbf{K})^{-1/2}\exp\left[\int d^d\mathbf{x}d^d\mathbf{x}'\frac{K^{-1}(\mathbf{x},\mathbf{x}')}{2}h(\mathbf{x})h(\mathbf{x}')\right],\end{aligned}\tag{II.63}$$

where the inverse kernel $K^{-1}(\mathbf{x},\mathbf{x}')$ satisfies

$$\int d^d\mathbf{x}'K(\mathbf{x},\mathbf{x}')K^{-1}(\mathbf{x}',\mathbf{x}'')=\delta^d(\mathbf{x}-\mathbf{x}'').\tag{II.64}$$

The notation $\mathcal{D}\phi(\mathbf{x})$ is used to denote the functional integral. There is a constant of proportionality, $(2\pi)^{N/2}$, left out of eq.(II.63). Although formally infinite in the continuum limit of $N\to\infty$, it does not effect the averages that are obtained as derivatives of such integrals. In particular, for Gaussian distributed functions, eq.(II.61) generalizes to

$$\begin{cases}\langle\phi(\mathbf{x})\rangle_c=\int d^d\mathbf{x}'K^{-1}(\mathbf{x},\mathbf{x}')h(\mathbf{x}')\\ \langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle_c=K^{-1}(\mathbf{x},\mathbf{x}')\end{cases}.\tag{II.65}$$

In dealing with small fluctuations to the Landau–Ginzburg Hamiltonian, we encountered the quadratic form

$$\int d^d\mathbf{x}[(\nabla\phi)^2+\phi^2/\xi^2]\equiv\int d^d\mathbf{x}d^d\mathbf{x}'\phi(\mathbf{x}')\delta^d(\mathbf{x}-\mathbf{x}')(-\nabla^2+\xi^{-2})\phi(\mathbf{x}),\tag{II.66}$$

which implies the kernel

$$K(\mathbf{x},\mathbf{x}')=K\delta^d(\mathbf{x}-\mathbf{x}')(-\nabla^2+\xi^{-2}).\tag{II.67}$$

Following eq.(II.64), the inverse kernel satisfies

$$K\int d^d\mathbf{x}''\delta^d(\mathbf{x}-\mathbf{x}'')(-\nabla^2+\xi^{-2})K^{-1}(\mathbf{x}''-\mathbf{x}')=\delta^d(\mathbf{x}'-\mathbf{x}),\tag{II.68}$$

which implies the differential equation

$$K(-\nabla^2+\xi^{-2})K^{-1}(\mathbf{x})=\delta^d(\mathbf{x}).\tag{II.69}$$

Comparing with eq.(II.44) implies $K^{-1}(\mathbf{x})=\langle\phi(\mathbf{x})\phi(\mathbf{0})\rangle=-I_d(\mathbf{x})/K$, as obtained before by a less direct method.

II.H Fluctuation Corrections to the Saddle Point

We can now examine how fluctuations around the saddle point solution modify the free energy, and other macroscopic properties. Starting with eq.(II.35), the partition function including small fluctuations is

$$Z \approx \exp\left[-V\left(\frac{t}{2}\bar{m}^2 + u\bar{m}^4\right)\right]\int \mathcal{D}\phi_\ell(\mathbf{x})\exp\left\{-\frac{K}{2}\int d^d\mathbf{x}\left[(\nabla\phi_\ell)^2 + \frac{\phi_\ell^2}{\xi_\ell^2}\right]\right\} \\ \cdot\int \mathcal{D}\phi_t(\mathbf{x})\exp\left\{-\frac{K}{2}\int d^d\mathbf{x}\left[(\nabla\phi_t)^2 + \frac{\phi_t^2}{\xi_t^2}\right]\right\}. \tag{II.70}$$

Each of the Gaussian kernels is diagonalized by the Fourier transforms

$$\tilde{\phi}(\mathbf{q}) = \int d^d\mathbf{x}\,\exp\left(-i\mathbf{q}\cdot\mathbf{x}\right)\phi(\mathbf{x})/\sqrt{V},$$

and with corresponding eigenvalues $K(\mathbf{q}) = K(q^2 + \xi^{-2})$. The resulting determinant of $\mathbf{K}$ is a product of such eigenvalues, and hence

$$\ln\det\mathbf{K} = \sum_{\mathbf{q}}\ln K(\mathbf{q}) = V\int\frac{d^d\mathbf{q}}{(2\pi)^d}\ln[K(q^2+\xi^{-2})]. \tag{II.71}$$

The free energy resulting from eq.(II.70) is then given by

$$f = -\frac{\ln Z}{V} = \frac{t\bar{m}^2}{2} + u\bar{m}^4 + \frac{1}{2}\int\frac{d^d\mathbf{q}}{(2\pi)^d}\ln[K(q^2+\xi_\ell^{-2})] + \frac{n-1}{2}\int\frac{d^d\mathbf{q}}{(2\pi)^d}\ln[K(q^2+\xi_t^{-2})]. \tag{II.72}$$

(Note that there are $n-1$ transverse components.) Using the dependance of the correlation lengths on reduced temperature, the singular part of the heat capacity is obtained as

$$C_{\text{singular}} \propto -\frac{\partial^2 f}{\partial^2 t} = \begin{cases} 0 + \dfrac{n}{2}\displaystyle\int\frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{(Kq^2+t)^2} & \text{for } t>0 \\ \dfrac{1}{8u} + 2\displaystyle\int\frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{(Kq^2-2t)^2} & \text{for } t<0 \end{cases}. \tag{II.73}$$

The correction terms are proportional to

$$C_F = \frac{1}{K^2}\int\frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{(q^2+\xi^{-2})^2}. \tag{II.74}$$

The integral has dimensions of $(\text{length})^{4-d}$, and changes behavior at $d=4$. For $d>4$ the integral diverges at large $\mathbf{q}$, and is dominated by the upper cutoff $\Lambda \simeq 1/a$, where a is the lattice spacing. For $d < 4$, the integral is convergent in both limits. It can be made dimensionless by rescaling $\mathbf{q}$ by ξ^{-1}, and is hence proportional to ξ^{4-d}. Therefore

$$C_F \simeq \frac{1}{K^2} \begin{cases} a^{4-d} & \text{for } d > 4 \\ \xi^{4-d} & \text{for } d < 4 \end{cases} . \qquad \text{(II.75)}$$

In dimensions $d > 4$, fluctuation corrections to the heat capacity add a constant term to the background on each side of the transition. However, the primary form of the singularity, a discontinuity in C, is not changed. For $d < 4$, the divergence of $\xi \propto t^{-1/2}$, at the transition leads to a correction term from eq.(II.75) which is more important than the original discontinuity. Indeed, the correction term corresponds to an exponent $\alpha = (4-d)/2$. However, this is only the first correction to the saddle point result. The diverge of C_F merely implies that the saddle point conclusions are no longer reliable in dimensions $d \leq 4$, called the *upper critical dimension*. Although we obtained this dimension by looking at the fluctuation corrections to the heat capacity, we would have reached the same conclusion in examining the singular part of any other quantity, such as magnetization or susceptibility. The contributions due to fluctuations always modify the leading singular behavior, and hence the critical exponents, in dimensions $d \leq 4$.

II.I The Ginzburg Criterion

We have thus established the importance of fluctuations, and identified them as the probable reason for the failure of the saddle point approximation to correctly describe the observed exponents. However, as noted in sec.II.G, there are some materials, such as superconductors, in which the experimental results are well fitted to the singular forms predicted by this approximation. Can we quantify why fluctuations are less important in superconductors than in other phase transitions?

Eq.(II.75) indicates that fluctuation corrections become important due to the divergence of the correlation length. Within the saddle point approximation, the correlation length diverges as $\xi \approx \xi_0 |t|^{-1/2}$, where $t = (T_c - T)/T_c$ is the reduced temperature, and $\xi_0 \approx \sqrt{K}$ is a *microscopic* length scale. In principal, ξ_0 can be measured experimentally from fitting scattering line shapes. It has to approximately equal the size of the units that undergo ordering at the phase transition. For the liquid–gas transition, ξ_0 can be estimated as $(v_c)^{1/3}$, where v_c is the critical atomic volume. In superfluids, ξ_0 is approximately the thermal wavelength $\lambda(T)$. Both these estimates are of the order of a few atomic spacings, 1–10Å. On the other hand, the underlying unit for superconductors is a Cooper pair. The paired electrons are forced apart by their Coulomb repulsion, resulting in a relatively large separation of $\xi_0 \approx 10^3$Å.

The importance of fluctuations can be gauged by comparing the two terms in eq.(II.73); the saddle point discontinuity $\Delta C_{\rm S.P.} \propto 1/u$, and the correction term C_F. Since $K \propto \xi_0^2$, the correction term is proportional to $\xi_0^{-d} t^{-(4-d)/2}$. Thus fluctuations are important provided,

$$\xi_0^{-d} t^{-\frac{4-d}{2}} \gg \Delta C_{\rm S.P.}, \quad \Longrightarrow \quad |t| \ll t_G \simeq \frac{1}{(\xi_0^d \Delta C_{\rm S.P.})^{\frac{2}{4-d}}}. \qquad \text{(II.76)}$$

The above requirement is known as the *Ginzburg criterion.* Naturally in $d < 4$, it is satisfied sufficiently close to the critical point. However, the resolution of the experiment may not be good enough to get closer than the Ginzburg reduced temperature t_G. If so, the apparent singularities at reduced temperatures $t > t_G$ may show saddle point behavior. It is this apparent discontinuity that then appears in eq.(II.76), and may be used to self–consistently estimate t_G. Clearly, $\Delta C_{\rm S.P.}$ and ξ_0 can both be measured in dimensionless units; ξ_0 in units of atomic size a, and $\Delta C_{\rm S.P.}$ in units of Nk_B. The latter is of the order of unity for most transitions, and thus $t_G \approx \xi_0^{-6}$ in $d = 3$. In cases where ξ_0 is a few atomic spacings, a resolution of $t_G \approx 10^{-1} - 10^{-2}$ will suffice. However, in superconductors with $\xi_0 \approx 10^3 a$, a resolution of $t_G < 10^{-18}$ is necessary to see any fluctuation effects. This is much beyond the ability of current apparatus. The newer ceramic high temperature superconductors have a much smaller coherence length of $\xi_0 \approx 10a$, and they indeed show some effects of fluctuations.

Again, it is worth emphasizing that a similar criterion could have been obtained by examining any other quantity. Fluctuations corrections become important in measurement of a quantity X for $t \ll t_G(X) \simeq A(X)\xi_0^{-2d/(4-d)}$. However, the coefficient $A(X)$ may be different (by one or two orders of magnitude) for different quantities. So, it is in principle possible to observe saddle point behavior in one quantity, while fluctuations are important in another quantity measured at the same resolution. Of course, fluctuations will always become important at sufficiently high resolutions.

A summary of the results obtained so far from the Landau–Ginzburg approach is as follows:

- For dimensions d greater than an upper critical dimension of $d_u = 4$, the saddle point approximation is valid, and singular behavior at the critical point is described by exponents $\alpha = 0$, $\beta = 1/2$, $\gamma = 1$, $\nu = 1/2$, $\cdots$.
- For d less than a lower critical dimensions ($d_\ell = 2$ for continuous symmetry, and $d_\ell = 1$ for discrete symmetry) fluctuations are strong enough to destroy the ordered phase.
- In the intermediate dimensions, $d_\ell \leq d \leq d_u$, fluctuations are strong enough to change the saddle point results, but not sufficiently important to completely destroy order. Unfortunately, or happily, this is the case of interest to us in $d = 3$.