Gaussian Integrals and The Hohenberg-Wagner-Mermin Theorem

The goal of these notes is to provide a basic understanding of how to do gaussian functional integrals as they come up in field theory. The ability to do gaussian integrals underlies the very successful apparatus of field theoretic perturbation which we will discuss in future notes. While developing the tools to do gaussian functional integrals, we will be able to justify the Hohenberg-Wagner-Mermin Theorem, which states that statistical models with a continuous symmetry can only spontaneously order at low temperatures in higher than 2 dimensions. These notes draw heavily on the book of Chaikin and Lubensky (sections 5.2 and 6.1), which I have found to be very helpful in understanding these things.

Warning: there may be some sign errors and missing factors of β in these notes.

1 Gaussian Integrals

1.1 The multivariate normal pdf

We will start with a review of the multivariate normal distribution, which can then be generalized with the appropriate limit to a continuous functional integral. If we have k gaussian random variables $\mathbf{X} \in \mathbb{R}^k$ with covariance matrix Σ defined by $\Sigma_{ij} = \langle X_i X_j \rangle$, their joint probability density function is given by

$$p_{\mathbf{X}}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^k \det \Sigma}} \exp\left[-\frac{1}{2}\mathbf{x}^\intercal \Sigma^{-1} \mathbf{x}\right] = \frac{1}{\sqrt{(2\pi)^k \det \Sigma}} \exp\left[-\frac{1}{2}\Sigma^{-1}_{ij} x_i x_j\right], \tag{1}$$

where repeated indices are summed. We will switch back and forth between vector and component notation as convenient. This formula above is a standard result, but how can we prove it?

First, let us check the validity of the normalization constant Z for the joint probability distribution of the $\{X_i\}$, defined as

$$Z = \int \exp\left[-\frac{1}{2}\mathbf{x}^\intercal \Sigma^{-1} \mathbf{x}\right] \prod_i dx_i. \tag{2}$$

In order to evaluate Z, we would like to write the expression in the integrand in terms of a diagonal matrix: this will recast our integral into a product of single-variable gaussian integrals. Since Σ is a covariance matrix and therefore symmetric and real, it admits orthogonal diagonalization and we can write $\Sigma = O^{-1}\Lambda O$ for Λ a diagonal matrix of the eigenvalues of Σ and O an orthogonal matrix such that $O^\intercal O^{-1}$. Therefore we can switch to integrating in variables $y_i = O_{ij} x_j$. The determinant of this transformation is 1 by orthogonality of the transformation, and so our desired integral can be written as

$$Z = \int \exp\left[-\frac{1}{2}\mathbf{y}^\intercal \Lambda^{-1} \mathbf{y}\right] \prod_i dy_i = (2\pi)^{k/2} \prod_{i=1}^{k} \Lambda_{ii}^{1/2} \tag{3}$$

where we have decoupled our integral into k independent gaussian integrals. Recalling that the Λ_{ii} are precisely the eigenvalues of Σ, we are left with the expression $\sqrt{(2\pi)^k \det \Sigma}$ for Z.

Now how do we show that $\langle X_i X_j \rangle = \Sigma_{ij}$? We can do so by a similar orthogonal transformation.

$$\langle X_i X_j \rangle = \frac{1}{Z} \int \exp\left[-\frac{1}{2}\mathbf{y}^\intercal \Lambda^{-1} \mathbf{y}\right] O^{-1}_{ik} y_k O^{-1}_{jl} y_l \prod_i dy_i. \tag{4}$$

Considering the term $O^{-1}_{ik} y_k O^{-1}_{jl} y_l = O^{-1}_{ik} O_{lj} y_k y_l$, we note that this is similar to the expression for $\Sigma_{ij} = [O^{-1}\Lambda O]_{ij} = O^{-1}_{ik}\Lambda_{kl} O_{lj}$. Now, using properties of single variable gaussian integrals (noting that Λ is diagonal), we have that

$$\frac{1}{Z} \int \exp\left[-\frac{1}{2}\mathbf{y}^\intercal \Lambda^{-1} \mathbf{y}\right] y_k y_l \prod_i dy_i = \Lambda_{kl}. \tag{5}$$

Therefore, putting these together, we have

$$\frac{1}{Z} \int \exp\left[-\frac{1}{2}\mathbf{y}^\intercal \Lambda^{-1} \mathbf{y}\right] O^{-1}_{ik} y_k O_{lj} y_l \prod_i dy_i = O^{-1}_{ik} \Lambda_{kl} O_{lj} = \Sigma_{ij}. \tag{6}$$

1.2 Completing the square

With this gaussian measure, we can calculate any moment of the $\{X_i\}$: all odd moments vanish, and even moments can be decomposed into two-point correlations with the help of Wick's (or Isserlis') theorem (which will be discussed in another set of notes). All the two point correlations follow directly from the covariance matrix Σ by definition.

We can also calculate integrals which involve exponentiating a linear function of the $\{x_i\}$, since these can be turned back into gaussian integrals by completing the square in the exponent. Namely,

$$\int \exp\left[-\frac{1}{2}\mathbf{x}^\intercal\Sigma^{-1}\mathbf{x} + \mathbf{u}\cdot\mathbf{x}\right]\prod_i dx_i = \sqrt{(2\pi)^k \det\Sigma} \times \exp\left[\frac{1}{2}\mathbf{u}^\intercal\Sigma\mathbf{u}\right], \tag{7}$$

since

$$\mathbf{x}^\intercal\Sigma^{-1}\mathbf{x} - 2\mathbf{u}\cdot\mathbf{x} = (\mathbf{x}^\intercal - \mathbf{u}\Sigma)\Sigma^{-1}(\mathbf{x} - \Sigma\mathbf{u}) - \mathbf{u}^\intercal\Sigma\mathbf{u}. \tag{8}$$

In statistical field theory, the energy of the system is a function of the field configuration, where this field can be a scalar or vector field. Therefore the partition function might look something like

$$Z = \int \mathcal{D}\phi(\mathbf{x})e^{-\beta\mathcal{H}}, \quad \text{with} \quad \mathcal{H} = \int d^d\mathbf{x}\left(r\phi(\mathbf{x})^2 + [\nabla\phi(\mathbf{x})]^2\right), \tag{9}$$

where in the simplest case $\phi(\mathbf{x})$ is a scalar field at every point in d-dimensional space. This field could represent an order parameter, as in the case of Landau theory for the Ising model, or it could be a microscopic angle field as in the XY model. We will see that this integral for the partition function is in fact a gaussian integral in disguise, and that we can therefore calculate much about correlations of the field $\phi(\mathbf{x})$ in thermal equilibrium.

2 Field Theory with a Quadratic Hamiltonian

2.1 Discrete space

We will first see how to evaluate the partition function of a field defined on a discrete lattice. Here we will adopt the notation of Chaikin and Lubensky, and be careful about distinguishing between lattice sites and positions. Imagine that $\phi(\mathbf{x})$ is only defined at lattice sites indexed by the vector $\mathbf{l}$. The lattice site $\mathbf{l}$ is at a position in space with coordinates $\mathbf{R}_\mathbf{l}$. We will use the shorthand $\phi(\mathbf{R}_\mathbf{l}) = \phi_\mathbf{l}$. Then a "harmonic" Hamiltonian — i.e. one that is quadratic in the fields $\{\phi_\mathbf{l}\}$ — has the form

$$\mathcal{H} = \frac{1}{2}\sum_{\mathbf{l},\mathbf{l}'} r_{\mathbf{l},\mathbf{l}'}\phi_\mathbf{l}\phi_{\mathbf{l}'}, \tag{10}$$

as long as we appropriately define the elements of the matrix r, given by $r_{\mathbf{l},\mathbf{l}'}$. Now if we want to evaluate

$$Z = \int \prod_\mathbf{l} d\phi_\mathbf{l} \exp\left[-\frac{\beta}{2}\sum_{\mathbf{l},\mathbf{l}'} r_{\mathbf{l},\mathbf{l}'}\phi_\mathbf{l}\phi_{\mathbf{l}'}\right], \tag{11}$$

where the integral is taken over the field at all the lattice sites [a discrete version of the functional integration measure $\mathcal{D}\phi(\mathbf{x})$], then we can recognize that this is a high-dimensional gaussian integral over a distribution of the type in Equation 1. *Note that from this form we can identify r with the inverse covariance matrix for the field at each of the lattice sites.*

In particular, if we could invert the matrix r, then we could calculate the partition function and all the correlation functions, since two point correlations would be given by $\langle\phi_\mathbf{l}\phi_{\mathbf{l}'}\rangle = \frac{1}{\beta}(r^{-1})_{\mathbf{l},\mathbf{l}'}$. If we could move into a basis where r is diagonal, then our job would be much easier. Then we could write $r = U\Lambda U^\dagger$ for diagonal matrix Λ containing the eigenvalues of r. We then have $r^{-1} = U\Lambda^{-1}U^\dagger$, and so the correlation functions can be calculated in terms of the eigenvalues and eigenvectors of the r matrix. How can we diagonalize r? The key will be to move into Fourier space.

Let us decompose ϕ into Fourier components, according to

$$\phi_\mathbf{l} = \sum_\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{R}_\mathbf{l}}\phi_\mathbf{q}. \tag{12}$$

Then we have

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{l},\mathbf{l}',\mathbf{q},\mathbf{q}'} r_{\mathbf{l},\mathbf{l}'} e^{i(\mathbf{q}\cdot\mathbf{R}_\mathbf{l} + \mathbf{q}'\cdot\mathbf{R}_{\mathbf{l}'})} \phi_\mathbf{q} \phi_{\mathbf{q}'}. \tag{13}$$

If we can write our Hamiltonian in the form

$$\mathcal{H} = \frac{1}{2} \sum_\mathbf{q} r(\mathbf{q}) |\phi_\mathbf{q}|^2, \tag{14}$$

then we see that this $r(\mathbf{q})$ matrix in Fourier space is diagonal. An arbitrary r matrix is not guaranteed to be diagonal in the Fourier basis, but many Hamiltonians of interest are: in particular if the Hamiltonian is translation invariant, with $r_{\mathbf{l},\mathbf{l}'}$ depending only on $|\mathbf{R}_\mathbf{l} - \mathbf{R}_{\mathbf{l}'}|$, then it will be diagonalizable in the Fourier basis [show this as an exercise, and find the relation between $r(\mathbf{q})$ and $r_{\mathbf{l},\mathbf{l}'}$]. Therefore the transformation of the ϕ variables in which r is diagonal is the discrete Fourier transform: the same one which sends $\phi_\mathbf{l}$ to $\phi_\mathbf{q}$. The matrix elements of this transformation (indexed by $\mathbf{l}$ and $\mathbf{q}$) are be given by $M_{\mathbf{lq}} = e^{i\mathbf{q}\cdot\mathbf{R}_\mathbf{l}}$, by the definition of the Fourier transform. This allows us to construct the matrix representation of a discrete Fourier transform as a change-of-basis matrix containing the eigenvectors of r.

We now have everything we need to calculate the correlation function $G_0(\mathbf{R}_\mathbf{l}, \mathbf{R}_{\mathbf{l}'}) = \langle \phi_\mathbf{l} \phi_{\mathbf{l}'} \rangle$. Namely,

$$G_0(\mathbf{R}_\mathbf{l}, \mathbf{R}_{\mathbf{l}'}) = \frac{1}{\beta} (r^{-1})_{\mathbf{l},\mathbf{l}'} = \frac{1}{\beta} \sum_\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{R}_\mathbf{l}} \frac{1}{r(\mathbf{q})} e^{-i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}'}}. \tag{15}$$

We can also directly calculate the partition function, which is proportional to the square root of the determinant of the r^{-1} matrix. Using the fact that $\det(A) = e^{\log\det(A)} = e^{\mathrm{Tr}\log(A)}$, for any matrix A, we have that

$$\log Z = \frac{1}{2} \log\left[\det\left(\frac{2\pi}{\beta} r^{-1}\right)\right] = \frac{1}{2} \sum_\mathbf{q} \log\left(\frac{2\pi}{\beta r(\mathbf{q})}\right). \tag{16}$$

Furthermore, if our Hamiltonian has terms which are linear in the the fields, of the form

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{l},\mathbf{l}'} r_{\mathbf{l},\mathbf{l}'} \phi_\mathbf{l} \phi_{\mathbf{l}'} - \sum_\mathbf{l} h_\mathbf{l} \phi_\mathbf{l}, \tag{17}$$

then we can use Equation 7 to see that

$$\log Z = \frac{1}{2} \sum_\mathbf{q} \log\left(\frac{2\pi}{\beta r(\mathbf{q})}\right) + \frac{\beta}{2} \sum_{\mathbf{l},\mathbf{l}'} h_\mathbf{l} G_0(\mathbf{R}_\mathbf{l}, \mathbf{R}_{\mathbf{l}'}) h_{\mathbf{l}'}, \tag{18}$$

where the expression for $G_0(\mathbf{R}_\mathbf{l}, \mathbf{R}_{\mathbf{l}'})$ is given in Equation 15.

2.2 Continuous space

Using this intuition from the discrete version, we can see that for $\phi(\mathbf{x})$ defined in continuous space, if our Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2} \int d^d\mathbf{x} d^d\mathbf{x}' r(\mathbf{x}, \mathbf{x}') \phi(\mathbf{x}) \phi(\mathbf{x}'), \tag{19}$$

and we can rewrite this as $\sum_\mathbf{q} r(\mathbf{q}) |\phi_\mathbf{q}|^2$, then our two-point correlations are given by

$$G_0(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle = \frac{1}{\beta(2\pi)^d} \int d^d\mathbf{q} \frac{e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}}{r(\mathbf{q})}. \tag{20}$$

In conjunction with Wick's theorem, this renders any harmonic Hamiltonian *exactly solvable*, in the sense that we can calculate any equilibrium properties of the field that we wish. We can also write down the partition function in the presence of fields which add a linear term to the Hamiltonian.

By analogy with the discrete case, the partition function for a Hamiltonian of form

$$\mathcal{H} = \frac{1}{2} \int d^d\mathbf{x} d^d\mathbf{x}' r(\mathbf{x}, \mathbf{x}') \phi(\mathbf{x}) \phi(\mathbf{x}') - \int d\mathbf{x} h(\mathbf{x}) \phi(\mathbf{x}) \tag{21}$$

is given by

$$\log Z = \frac{1}{2}\int \frac{d^d q}{(2\pi)^d} \log\left(\frac{2\pi}{\beta r(\mathbf{q})}\right) + \frac{\beta}{2}\int d^d x d^d x' h(\mathbf{x}) G_0(\mathbf{x},\mathbf{x}') h(\mathbf{x}'), \tag{22}$$

with correlation function $G_0(\mathbf{x},\mathbf{x}')$ given in Equation 20. Note that in this case with the fields, the correlation $\langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle$ will be different from the case of zero field, due to the nonzero mean of the field values: but if we subtract off their means to get the covariance, this will be the same with and without a field.

3 The Hohenberg-Wagner-Mermin Theorem

While building the machinery to do gaussian integrals in the limit of infinite numbers of variables, we have developed the necessary tools to illustrate the Hohenberg-Wagner-Mermin (HWM) Theorem, which states that in 2 dimensions or lower, a continuous symmetry cannot be broken by spontaneous ordering of a field. What does this mean? If we have a statistical field that has a continuous degree of freedom, then this field will *not* spontaneously order at low enough temperatures. Note that the 2D Ising model does not have a continuous symmetry and therefore this theorem does not apply: indeed it is known that the 2D Ising model exhibits a phase transition at finite temperature. However, for the XY model in which spins are modeled as 2 dimensional vectors with a continuous rotational symmetry, the theorem applies and correctly states that there is no long range order at low temperatures.

3.1 Heuristic explanation

We can give an intuitive explanation of the HWM theorem with a scaling argument. Consider a system of dimension d and size L in each dimension, with a continuous symmetry. For example, in the XY model, this symmetry corresponds to a uniform rotation of all the spins. Since the spins take on continuous values, there can be very low energy excitations that span the length of the system. In particular, one could imagine a configuration in which θ increases from 0 to 2π across the length of the whole system, meaning that θ at neighboring sites would differ by $2\pi/L$. The energy of such an excitation between two neighboring spins is then $(2\pi/L)^2$. Integrated over the whole system, the energy scales as L^d/L^2. Therefore for only for $d > 2$ does the energy of a low lying excitation get large in the thermodynamic limit. Otherwise the energy of a the lowest energy excitation approaches 0 in the thermodynamic limit, and can therefore be excited arbitrarily close to 0 temperature. When the energy of the lowest energy excitations increases with system size at low temperatures, symmetry breaking occurs, since the system cannot realize these excitations.

3.2 The XY Model

The XY model is a model of interacting magnetic spins on a lattice, where the spins are confined to point in a two dimensional subspace of the lattice dimension. [Though we introduce it as a magnetism model, the XY model is widely relevant in the study of superconductors and superfluids, where the order parameters are complex numbers characterized by a phase similar to the angle θ here.] In our case will consider the XY model in 2 dimensions, where the spins are of unit length oriented in the plane of the lattice. Each spin $\mathbf{s}_i$ is therefore characterized by an angle θ_i, and the Hamiltonian for the model is

$$\mathcal{H}_{XY} = -\frac{K}{2}\sum_{\langle ij\rangle} \mathbf{s}_i\cdot\mathbf{s}_j = -\frac{K}{2}\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j), \tag{23}$$

where $\mathbf{s}_i = (\cos(\theta_i), \sin(\theta_i))$.

We can further substantiate the general argument of the preceding section as follows: If our scalar field, which we will call θ, is continuous variable of space (for example the angle field in the XY model), it means that our Hamiltonian (at low temperatures) contains a term like $\int d^d\mathbf{x}(\nabla\theta(\mathbf{x}))^2$. This is not be confused with a similar looking term in the Hamiltonian for the Ising model, in which the spins are intrinsically *discrete*. In the latter expression ϕ is usually used instead of θ, and it represents the order parameter field: a macroscopic quantity which is the average magnetization. However in the XY model θ is the microscopic angle. Without an external field, the Hamiltonian of the XY model for small angle fluctuations can be Taylor expanded to read

$$\mathcal{H}_{XY} \approx \frac{K}{2}\int d^d\mathbf{x}[\nabla\theta(\mathbf{x})]^2 = \frac{K}{2}\sum_{\mathbf{q}} q^2|\theta_{\mathbf{q}}|^2. \tag{24}$$

From earlier, we already know how to calculate the partition function from this Hamiltonian! We are also interested in calculating correlations of the form $\langle\cos[\theta(\mathbf{x}) - \theta(\mathbf{x}')]\rangle = \mathrm{Re}\langle e^{i(\theta(\mathbf{x})-\theta(\mathbf{x}'))}\rangle$, which represent the correlation functions of the spins in the model. To calculate this expectation, we wish to evaluate

$$\langle e^{i(\theta(\mathbf{x})-\theta(\mathbf{x}'))}\rangle = \frac{1}{Z}\int \mathcal{D}\theta(\mathbf{x}) e^{-\beta\mathcal{H}_{XY}} e^{i(\theta(\mathbf{x})-\theta(\mathbf{x}'))} \text{ with } Z = \int \mathcal{D}\theta(\mathbf{x}) e^{-\beta\mathcal{H}_{XY}}. \tag{25}$$

The integral here can be written as

$$\int \mathcal{D}\theta(\mathbf{x}) \exp\left[-\beta\left(\mathcal{H}_{XY} - \frac{i}{\beta}(\theta(\mathbf{x}) - \theta(\mathbf{x}'))\right)\right]. \tag{26}$$

We see that this integral can be evaluated by considering the contribution $\frac{i}{\beta}(\theta(\mathbf{x}) - \theta(\mathbf{x}'))$ as a field $h(\mathbf{y}) = \frac{i}{\beta}[\delta(\mathbf{y}-\mathbf{x}) - \delta(\mathbf{y}-\mathbf{x}')]$.

Plugging this form of $h(\mathbf{y})$ into Equation 22, and noting that the factor of Z cancels out gives

$$\log\langle e^{i(\theta(\mathbf{x})-\theta(\mathbf{x}'))}\rangle = -\frac{1}{2\beta}\int d^dy d^dy' [\delta(\mathbf{y}-\mathbf{x}) - \delta(\mathbf{y}-\mathbf{x}')] G_0(\mathbf{y},\mathbf{y}')[\delta(\mathbf{y}'-\mathbf{x}) - \delta(\mathbf{y}'-\mathbf{x}')] \tag{27}$$

$$= -\frac{1}{\beta}\int \frac{d^dq}{(2\pi)^d}\frac{1-e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}}{q^2}. \tag{28}$$

where we used the fact that

$$G_0(\mathbf{x},\mathbf{x}') = \frac{1}{\beta(2\pi)^d}\int d^d\mathbf{q}\frac{e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}}{q^2}. \tag{29}$$

This expression for the spin correlation function can be evaluated: the important point is that the results depends strongly on the dimension d. For $d = 1$ we find that $\langle e^{i(\theta(\mathbf{x})-\theta(\mathbf{x}'))}\rangle$ is decaying exponentially. For $d = 2$ it decays algebraically, with a power law whose exponent depends on the inverse temperature β. For $d = 3$ and above $\langle e^{i(\theta(\mathbf{x})-\theta(\mathbf{x}'))}\rangle$ asymptotes to a nonzero value for $|\mathbf{x}-\mathbf{x}'| \to \infty$, indicating spontaneous symmetry breaking and long range order.

The decay of the correlation function in $d = 1$ and $d = 2$ indicates that there can be no long range ordering as long as the energy of the field has a term that looks like $[\nabla\theta]^2$, which will be the case when there is a continuous symmetry. The algebraic decay in $d = 2$ indicates that this is a marginal dimension; indeed $d = 2$ is special for the XY model, and the low-temperature transition that takes place does not fit into the conventional spontaneous symmetry breaking paradigm.

At high temperatures the expansion of $\cos(\theta_i - \theta_j)$ that we performed is no longer valid, and the periodicity of θ becomes important. There is a transition to a phase where the spin correlation function decays exponentially even in $d = 2$. The contribution of Kosterlitz and Thouless was to understand why and when this low temperature expansion [where we can approximate the Hamiltonian as being proportional to $\int(\nabla\theta)^2$] stops working, and to analyze (using renormalization group) the transition into the phase where excitations in the θ field, or *topological defects*, proliferate and destroy the algebraic order.

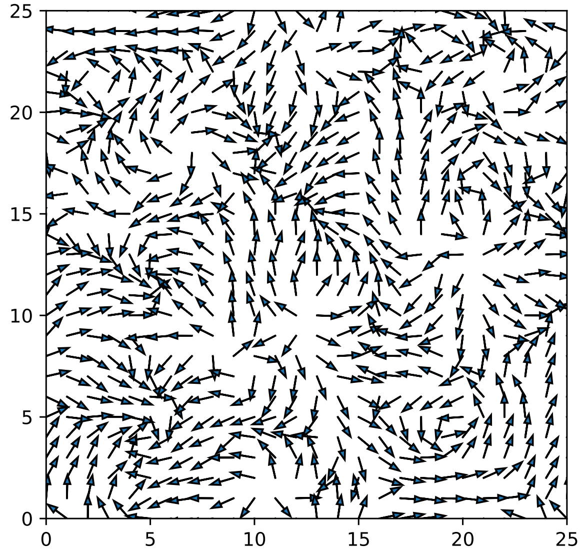

Figure 1: Vortices in the XY model, visible as defects where the orientation of the spin field is undefined.

4 References

Principles of Condensed Matter Physics: Chaikin and Lubensky: sections 5.2, 6.1
Wikipedia article on HWM theorem