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Chapter 1

Broken Symmetry

1.1 Introduction

What is the world made of? To a philosopher, this question lies at the intersection of ontology (the 'study' of being and existence) and mereology (the 'study' of parts and wholes). To a physicist, the answer very much depends on whom you ask, because ultimately it is a matter of energy scales. To a condensed matter physicist, the world consists of electrons, nuclei, and photons. That's pretty much it¹. The characteristic energy scales in condensed matter typically range from milli-electron volts (meV) to electron volts (eV)². By contrast, the protons and neutrons which constitute nuclei typically have binding energies on the order of MeV. The nucleons themselves consist of quarks and gluons. Quarks acquire their masses from coupling to the Higgs field, but some 99% of the nucleon mass is due to gluons and virtual quark-antiquark pairs, *i.e.* to the physics of QCD binding³.

1.1.1 The mother of all Hamiltonians

The Hamiltonian for a single electron in the presence of a static external potential $V(\mathbf{r})$ and electromagnetic vector potential $\mathbf{A}(\mathbf{r})$ is given by

$$H = \frac{\pi^2}{2m} + V(\mathbf{r}) + \frac{e\hbar}{2mc}\,\boldsymbol{\sigma}\cdot\boldsymbol{H} + \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}V \times \boldsymbol{\pi} + \frac{\hbar^2}{8m^2c^2}\boldsymbol{\nabla}^2V + \frac{(\pi^2)^2}{8m^3c^2} + \dots , \qquad (1.1)$$

¹Sometimes experimentalists use muons or even positrons to probe their samples, but the samples themselves consist of electrons and nuclei.

²Sometimes higher energy probes on the order of keV are used, for example in photoemission spectroscopy.

³So the next time you overhear someone holding forth about how the Higgs field (or, worse still, the Higgs boson) gives mass to everything in the universe, you can tell them that they are full of shit.



Figure 1.1: What is the world made of? It depends on whom you ask.

where $\pi = p + \frac{e}{c}A$. Where did this come from? From the Dirac equation,

$$i\hbar \frac{\partial \Psi}{\partial t} = \begin{pmatrix} mc^2 + V & c \,\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \\ c \,\boldsymbol{\sigma} \cdot \boldsymbol{\pi} & -mc^2 + V \end{pmatrix} \Psi = E\Psi \,. \tag{1.2}$$

The wavefunction Ψ is a four-component Dirac spinor. Since mc^2 is the largest term for our applications, the upper two components of Ψ are essentially the positive energy components. However, the Dirac Hamiltonian mixes the upper two and lower two components of Ψ . One can 'unmix' them by making a canonical transformation,

$$H \longrightarrow \hat{H}' \equiv e^{iS} \hat{H} e^{-iS} , \qquad (1.3)$$

where *S* is Hermitian, to render \hat{H}' block diagonal. With $E = mc^2 + \varepsilon$, the effective Hamiltonian is given by (1.1). This is known as the Foldy-Wouthuysen transformation, the details of which may be found in many standard books on relativistic quantum mechanics and quantum field theory (*e.g.* Bjorken and Drell, Itzykson and Zuber, *etc.*) and are recited in §1.6 below. Note that the Dirac equation leads to g = 2. If we go beyond "tree level" and allow for radiative corrections within QED, we obtain a perturbative expansion,

$$g = 2\left\{1 + \frac{\alpha}{2\pi} + \mathcal{O}(\alpha^2)\right\},\tag{1.4}$$

	6	
הסיכום	<u>Summary</u>	
הוגה אחד זקן מחדרו אל תלמידיו יצא ואמר בנקשו במקל: שמעו אחרון דברי אשר אשא כי הגיע הזמן לסכם, לאחר שנות בינה ועיצה, מה הם, לסוף מיצוי, הדברים שמהם העולם עשוי.	One old thinker out from his chamber to his disciples came and he said as he rapped with his cane: harken to the last of my words for it is now time to summarize, after years of reason and deliberation, what, in the last analysis, are the things of which the world is made.	e Natan Alterman (1910 - 1970)
העולם, נכבדי – שאחרי כל תהיות ופליאות בו דברי אמורים – עשוי ארץ, שמים, שיחים, סנוניות, אוניות, גלי ים, נהרות, ערים גדולות וקטנות, ירידים, צנוניות, כל מיני פטישים, נייר, משורים, רחובות, חדרים, – כך הוסיף למנות	The world, my distinguished sirs – which a and marveling my words concern – is made of land, sky, bushes, sparrows, ships, waves, rivers, cities large and small, fairs, radishes, all kinds of hammers, paper, saws, streets, rooms - thus he continued countin	fter all wondering
ולמנות – גאיות, שפלות, הרים וגבעות – ושעה שרופא ואחות כבר עליו גחנו בבית–החולים, עדיין היו שפתיו נעות ומונות – קלחות, כפיות, ספרים, מגרות, צנצנות – ומילים אחרונות שהשמיע היו: נעצים, כפתורים.	and counting – valleys, plains, mountains, hills – and while the doctor and nurse were bent over him in the hospital, still his lips were moving and counting – cauldrons, spoons, books, drawers, jars – and the last words which he uttered were: thumbtacks, buttor	ıs.
	(translatio	n by Assa Auerbach)

Figure 1.2: What is the world made of? Another point of view.

where $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant⁴.

There are two terms in (1.1) which involve the electron's spin:

Zeeman interaction :
$$\hat{H}_{Z} = \frac{e\hbar}{2mc} \boldsymbol{\sigma} \cdot \boldsymbol{H}$$

Spin-orbit interaction : $\hat{H}_{SO} = \frac{\hbar}{4m^{2}c^{2}} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V \times \left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)$. (1.5)

The numerical value for $\mu_{\scriptscriptstyle\rm B}$ is

$$\mu_{\rm B} = \frac{e\hbar}{2mc} = 5.788 \times 10^{-9} \,\text{eV/G}$$

$$\mu_{\rm B}/k_{\rm B} = 6.717 \times 10^{-5} \,\text{K/G} \quad .$$
(1.6)

⁴Note that with $\mu_n = e\hbar/2m_pc$ for the nuclear magneton, $g_p = 2.793$ and $g_n = -1.913$. These results immediately suggest that there is composite structure to the nucleons, *i.e.* quarks.

So on the scale of electron volts, laboratory scale fields ($H \lesssim 10^6$ G) are rather small (and ~2000 times smaller for nucleons).

In condensed matter, the potential $V(\mathbf{r})$ for the electron is a sum of terms from individual ion cores, *i.e.* $V(\mathbf{r}) = \sum_{a} v_a(\mathbf{r} - \mathbf{R}_a)$ where $v_a(\mathbf{r})$ is the atomic potential and \mathbf{R}_a is the location of the a^{th} nucleus. For Coulomb interactions, $v_a(\mathbf{r}) = -Z_a e^2/r$. The ion cores interact as well, with a potential $u_{ab}(\mathbf{r}) = Z_a Z_b e^2/r$. Putting it all together, we have⁵

$$\mathcal{H} = \sum_{i} \frac{\pi_{i}^{2}}{2m} - \frac{e\hbar}{2mc} \mathbf{H} \cdot \sum_{i} \boldsymbol{\sigma}_{i} - \sum_{i < j} \frac{e^{2}}{|\mathbf{r}_{i} - \mathbf{r}_{j}|} + \sum_{i,a} v_{a}(\mathbf{r}_{i} - \mathbf{R}_{a}) + \frac{\hbar}{4m^{2}c^{2}} \sum_{i,a} \boldsymbol{\sigma}_{i} \cdot \boldsymbol{\nabla}_{i} v_{a}(\mathbf{r}_{i} - \mathbf{R}_{a}) \times \boldsymbol{\pi}_{i} + \sum_{a} \frac{\boldsymbol{\Pi}_{a}^{2}}{2M_{a}} + \sum_{a < b} u_{ab}(\mathbf{R}_{a} - \mathbf{R}_{b}) \quad ,$$

$$(1.7)$$

with $\Pi_a = P_a - Z_a e A(R_a)/c$, and subject to the commutation relations,

$$\left[p_{i}^{\alpha}, r_{j}^{\beta}\right] = -i\hbar\delta_{ij}\delta^{\alpha\beta} \quad , \quad \left[P_{a}^{\alpha}, R_{b}^{\beta}\right] = -i\hbar\delta_{ab}\delta^{\alpha\beta} \quad , \quad \left[\sigma_{i}^{\mu}, \sigma_{j}^{\nu}\right] = 2i\delta_{ij}\epsilon^{\mu\nu\lambda}\sigma_{i}^{\lambda} \quad . \tag{1.8}$$

We may call Eqn. 1.7 the Mother of all Hamiltonians.

In a crystal, we may write $\mathbf{R}_a = \mathbf{R}_a^0 + \delta \mathbf{R}_a$, where $\{\mathbf{R}_a^0\}$ are the mean locations of the ion cores. These form a regular lattice. The deviations $\delta \mathbf{R}_a$ describe quantum mechanical fluctuations about the fixed crystalline coordinates. The quantized vibrations of a crystalline lattice are called *phonons*. Thus, the mother of all Hamiltonians describes electrons, which possess quantized spin, interacting among themselves and with fluctuating ion cores.

1.2 Classical and Quantum Statistical Physics

While the Mother of all Hamiltonians is too complex for us to attack directly, progress can oftentimes be made by examining parts of it, such as the spectrum of lattice vibrations, or the electronic energy spectrum in the presence of a crystalline lattice potential, possibly including spin-orbit effects. For such noninteracting systems, where the Hamiltonian is quadratic in electron or phonon operators, we can often go quite far in obtaining complete solutions. The problem becomes complicated when we consider the effects of *quenched impurities*, such as vacancies or substitutional defects in the crystalline lattice, which are random in nature. We must then consider how observable quantities are distributed with respect to an *ensemble* of configurations of the randomness. This can give rise to interesting, robust, and fundamentally new possibilities, such as localization.

In order to account for phonon-phonon, electron-phonon, and/or electron-electron interactions, there are few useful techniques at our disposal. We can always resort to perturbation

⁵We drop the last two and all following terms in Eqn. 1.1.

theory in the interactions, but this can lead us astray if the true ground state of the interacting system lies on the other side of a phase boundary from the noninteracting ground state. For gapless systems, such as metals, the situation is particularly tricky and we generally have no good reason why perturbation theory should converge⁶.

Suppose we have an idealized system described by a model Hamiltonian H which is simpler than \mathcal{H} and where we might hope to make some progress. The thermodynamic properties of the system are calculable from the Helmholtz free energy $F = -k_{\rm B}T \ln \operatorname{Trexp}(-H/k_{\rm B}T)$ or one of its Legendre transforms, such as the grand potential $\Omega = -k_{\rm B}T \ln \operatorname{Trexp}(-K/k_{\rm B}T)$, where $K = H - \mu N$. We write the Hamiltonian as

$$H = H_0 - \sum_{\alpha} h_{\alpha} Q_{\alpha} \quad , \tag{1.9}$$

where Q_{α} is a Hermitian operator and h_{α} is a conjugate field for each index α . Then the free energy *F* is a function of the fields, *i.e.* $F = F(\{h_{\alpha}\})$ and we have that the thermodynamic average of Q_{α} is

$$\langle Q_{\alpha} \rangle = -\frac{\partial F}{\partial h_{\alpha}}$$
 (1.10)

One can now define the *susceptibility*

$$\chi_{\alpha\beta} = \frac{\partial \langle Q_{\alpha} \rangle}{\partial h_{\beta}} = -\frac{\partial^2 F}{\partial h_{\alpha} \partial h_{\beta}} \quad . \tag{1.11}$$

Dynamical responses are defined for Hamiltonians of the form

$$H(t) = H_0 - \sum_{\alpha} h_{\alpha}(t) Q_{\alpha}$$
 (1.12)

Time-dependent first order perturbation theory then yields

$$\left\langle Q_{\alpha}(t)\right\rangle = \int_{-\infty}^{\infty} dt' \,\chi_{\alpha\beta}(t-t') \,h_{\beta}(t') + \mathcal{O}(h^2) \tag{1.13}$$

with

$$\chi_{\alpha\beta}(t-t') = \frac{i}{\hbar} \left\langle \left[Q_{\alpha}(t), Q_{\beta}(t') \right] \right\rangle \Theta(t-t') \quad .$$
(1.14)

⁶Oftentimes in quantum field theory, perturbation theory yields an *asymptotic series* in the coupling parameter(s). In this case the series expansions for physical quantities may be formally divergent, but provided the couplings are not too large, yield better and better approximations up until a particular order in the expansion. For example, in quantum electrodynamics, the relevant coupling is the fine structure constant $\alpha = e^2/\hbar c \approx 1/137$, and perturbation theory, typically evaluated using Feynman diagrams, is expected to start diverging at order α^{-1} .

⁷Also called the Landau free energy.

Note that the response is *causal*, *i.e.* the value of $\langle Q_{\alpha}(t) \rangle$ depends only on the values of $\{h_{\beta}(t')\}$ for t' < t. The *spectral representation* of the response function $\chi_{\alpha\beta}(t-t')$ is defined via its Fourier transform,

$$\hat{\chi}_{\alpha\beta}(\omega+i\epsilon) \equiv \frac{i}{\hbar} \int_{0}^{\infty} dt \left\langle \left[Q_{\alpha}(t), Q_{\beta}(0)\right] \right\rangle e^{i\omega t} e^{-\epsilon t}$$

$$= \frac{1}{\hbar Z} \sum_{m,n} e^{-\beta E_{m}^{0}} \left\{ \frac{\left\langle m \mid Q_{\beta} \mid n \right\rangle \left\langle n \mid Q_{\alpha} \mid m \right\rangle}{\omega + (E_{n}^{0} - E_{m}^{0})/\hbar + i\epsilon} - \frac{\left\langle m \mid Q_{\alpha} \mid n \right\rangle \left\langle n \mid Q_{\beta} \mid m \right\rangle}{\omega - (E_{n}^{0} - E_{m}^{0})/\hbar + i\epsilon} \right\} ,$$

$$(1.15)$$

where $Z = \text{Tr} \exp(-H_0/k_{\text{B}}T)$ and where $H_0 |n\rangle = E_n^0 |n\rangle$.

Finally, the indices α and β may be appended by spatial coordinates in the case of local operators $Q_{\alpha}(\mathbf{r})$, in which case we write

$$H(t) = H_0 - \sum_{\alpha} \int d^d r \ h_{\alpha}(\mathbf{r}, t) \ Q_{\alpha}(\mathbf{r}) \quad .$$
(1.16)

For example, $Q_{\alpha}(\mathbf{r})$ could be taken to be the local density $n(\mathbf{r})$ or a component $S^{\alpha}(\mathbf{r})$ of the local spin density. One then defines the response function

$$\chi_{\alpha\beta}(\mathbf{r},t \,|\, \mathbf{r};,t') \equiv \frac{\delta \langle Q_{\alpha}(\mathbf{r},t) \rangle}{\delta h_{\beta}(\mathbf{r}',t')} \quad .$$
(1.17)

1.2.1 Correspondence between quantum and classical statistical mechanics

In classical statistical physics, in systems where spontaneous symmetry breaking results in an ordered phase in which the local order parameter field takes on a finite average, *i.e.* $\langle \phi(\mathbf{r}) \rangle \neq 0$, the connected correlation function at large distances in the vicinity of the transition behaves as (for *r* fixed and $T \rightarrow T_c$)

$$C(\mathbf{r},T) = \left\langle \phi(\mathbf{r}) \,\phi(\mathbf{0}) \right\rangle - \left\langle \phi(\mathbf{r}) \right\rangle \left\langle \phi(\mathbf{0}) \right\rangle \sim A \, r^{2-d} \, e^{-r/\xi} \quad , \tag{1.18}$$

where $\xi(T) \sim |T - T_c|^{-\nu}$ is the spatial correlation length and ν the correlation length exponent⁸. Pretty much all classical phase transitions are described by a continuum field theory of sorts, with a free energy functional

$$F[\boldsymbol{\phi}(\boldsymbol{r})] = \int d^d x \, f(\boldsymbol{\phi}, \boldsymbol{\nabla} \boldsymbol{\phi}) \quad . \tag{1.19}$$

⁸Precisely at $T = T_c$, the correlation function behaves as $\langle \phi(\mathbf{r}) \phi(\mathbf{0}) \rangle \sim r^{-(d-2+\eta)}$, where η is the so-called *anomalous dimension*.

Here $\phi(\mathbf{x}) = \{\phi^1, \dots, \phi^N\}$ is an *N*-component real field, and by $\nabla \phi$ we mean the set of dN first derivatives $\partial \phi^a / \partial x^i$ with $a \in \{1, \dots, N\}$ and $i \in \{1, \dots, d\}$. The partition function is given by the functional integral

$$Z = \int D\phi(\mathbf{r}) e^{-F[\phi(\mathbf{r})]} \quad . \tag{1.20}$$

For the Ising model, one generally has N = 1 and one may take

$$f_{\text{Ising}}(\phi, \nabla \phi) = \frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} a \phi^2 + \frac{1}{4} b \phi^4 \quad , \tag{1.21}$$

i.e. a scalar ϕ^4 theory in *d* dimensions.

For bosonic quantum systems, the path integral formulation results in the following prescription. The partition function is once again given by a functional integral,

$$Z = \int D\phi(\mathbf{r},\tau) e^{-S_{\mathsf{E}}[\phi(\mathbf{r},\tau)]} \quad , \tag{1.22}$$

but now the field $\phi(\mathbf{r}, \tau)$ is dependent both on spatial coordinates \mathbf{r} as well as a "Euclidean time" coordinate $\tau \in [0, \hbar/k_{\text{B}}T]$, where T is the temperature. $S_{\text{E}}[\phi]$ is the *Euclidean action*,

$$S_{\mathsf{E}}[\boldsymbol{\phi}(\boldsymbol{r},t)] = \int_{0}^{\hbar\beta} d\tau \int d^{d}x \, \mathcal{L}_{\mathsf{E}}(\boldsymbol{\phi}, \boldsymbol{\nabla} \boldsymbol{\phi}, \partial_{\tau} \boldsymbol{\phi}) \quad , \qquad (1.23)$$

where $\mathcal{L}_{\mathsf{E}}(\phi, \nabla\phi, \partial_{\tau}\phi)$ is the *Euclidean Lagrangian density*. Note that spacetime consists of a 'slice' of finite temporal width $\hbar/k_{\text{B}}T$. If we define the coordinate $x^0 \equiv c\tau$, where c is a (possibly arbitrary) constant with dimensions of velocity, then we see that the action is given by a (d+1)-dimensional integral over a slab of finite width $L_{\tau} = c\tau/k_{\text{B}}T$ in the x^0 dimension. Hence the oft-heard maxim, *quantum mechanics in d (space) dimensions is equivalent to classical statistical mechanics in (d+1) dimensions*. While this is essentially true, it may be the case, as we emphasize below, that the resulting (d + 1)-dimensional classical model derived from a given quantum theory will be *anisotropic* in that the x^0 direction is special, both due to its finite extent for T > 0 systems and also due to the form of the derivative terms in the Lagrangian density. Indeed, nonrelativistic quantum theories generally result in such anisotropic classical models, although an emergent low-energy relativistic symmetry is sometimes present for particular systems, such as quantum antiferromagnets or acoustic phonons, or perhaps in the vicinity of a quantum critical point, such as near the tips of the 'Mott lobes' of the Bose Hubbard model.

For bosonic systems, $\phi(\mathbf{r}, \tau)$ may be taken to be an *N*-component real field, or a complexified version thereof⁹. As an example of a Euclidean Lagrangian density, consider the case

$$\mathcal{L}_{\mathsf{E}}(\boldsymbol{\phi}, \boldsymbol{\nabla} \boldsymbol{\phi}, \partial_{\tau} \boldsymbol{\phi}) = \frac{1}{2} \left(\frac{\partial \boldsymbol{\phi}}{\partial \tau} \right)^2 + \frac{1}{2} K(\boldsymbol{\nabla} \boldsymbol{\phi})^2 + V(\boldsymbol{\phi}) \quad .$$
(1.24)

⁹For example $(\phi^1, \phi^2) \rightarrow \phi \equiv \phi^1 + i\phi^2$.



Figure 1.3: Spatial and temporal correlations in the vicinity of a quantum phase transition. (The parameter *c* carries dimensions of velocity and may be arbitrary.)

This model may possess various discrete or continuous symmetries. For example, if we let $g \in O(N)$ be an arbitrary rotation in the internal space of the field ϕ , and if $V(g\phi) = V(\phi)$ for all such g, then the model is said to possess an O(N) symmetry (which may be broken - see below. Another important symmetry of the model is the O(d + 1) symmetry resulting from mixing space and time coordinates (with appropriate rescaling so as to render them of the same dimension). The *real time* correlations of this model will then exhibit a Lorentz symmetry. But not all QFTs have such a relativistic symmetry. Consider the case N = 2, for example, with

$$\mathcal{L}_{\mathsf{E}}(\boldsymbol{\phi}, \boldsymbol{\nabla} \boldsymbol{\phi}, \partial_{\tau} \boldsymbol{\phi}) = i \phi_1 \partial_{\tau} \phi_2 - i \phi_2 \partial_{\tau} \phi_1 + \frac{1}{2} K(\boldsymbol{\nabla} \boldsymbol{\phi})^2 + V(\boldsymbol{\phi}^2) \quad . \tag{1.25}$$

Here $\phi = (\phi_1, \phi_2)$. The 'kinetic' term is only linear in time derivatives, while the spatial derivative terms appear quadratically. This model has no relativistic symmetry, but it does have a global O(2) symmetry.

For fermionic systems, one also has a path integral, but it is over anticommuting Grassmann fields $\psi_{\sigma}(\mathbf{r},t)$ and their conjugates $\bar{\psi}_{\sigma}(\mathbf{r},\tau)$, which we shall discuss in due time¹⁰. An example might be

$$\mathcal{L}_{\mathsf{E}}(\psi_{\sigma},\bar{\psi}_{\sigma},\nabla\psi_{\sigma},\nabla\bar{\psi}_{\sigma},\partial_{\tau}\psi_{\sigma},\partial_{\tau}\bar{\psi}_{\sigma}) = \bar{\psi}_{\sigma}\Big(\hbar\partial_{\tau}-\mu-\frac{\hbar^{2}}{2m}\nabla^{2}\Big)\psi_{\sigma}+U\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\psi_{\downarrow}\psi_{\uparrow}$$
(1.26)

Note that the Laplacian term may be spatially integrated by parts to yield a term proportional to $\nabla \bar{\psi}_{\sigma} \cdot \nabla \psi_{\sigma}$. This \mathcal{L}_{E} corresponds to the Hubbard model.

As we approach a quantum phase transition, which occurs at temperature T = 0 and a critical value $g = g_c$ of some coupling, the spatial correlation length $\xi(g)$ grows as $\xi(g) \sim |g - g_c|^{-\nu}$. For systems with relativistic invariance, the correlation length in the imaginary time direction

¹⁰Real time, rest assured.

 $\xi_{\tau}(g)$ behaves in the same way, *i.e.* with the same correlation length exponent. But in general, the temporal exponent is different and may be written as $\nu_{\tau} = z\nu$, where *z* is the *dynamic critical exponent*. Thus, $\xi_{\tau}(g) \sim |g - g_c|^{-z\nu}$. As $g \to g_c$, both $\xi(g)$ and $\xi_{\tau}(g)$ will diverge. But at finite temperature, the width of the time slice is finite, given by $\hbar/k_{\rm B}T$. Thus, when *g* is sufficiently close to g_c such that $\xi_{\tau}(g) \gg L_{\tau} = \hbar c/k_{\rm B}T$, where *c* is an arbitrary measure of velocity, the fields will be 'locked' in the imaginary time direction. In this case, the expression for the partition function reverts to the classical result. What this tells us is that *quantum mechanics is irrelevant at any finite temperature T*, *i.e.* QM does not change the critical exponents at any finite temperature phase transitions. It should be emphasized that the above argument presumes the existence of a local order parameter field $\phi(\mathbf{r})$ whose correlations asymptotically decay on the scale of the correlation length $\xi(g, T)$. In the case of topological phases, where there is no such local order parameter, this argument may not apply.

1.3 Phases of matter

Condensed matter physicists are not interested in electrons, nuclei, and photons in isolation. Rather it is the collective properties of these interacting constituents which leads to the remarkably rich phenomenology of condensed matter. This richness is manifested by the bewildering array of *phases of matter* that can be conjured. Until relatively recently, phases of matter were described based on the *Landau paradigm*, in which an ordered phase is described by one or more nonzero *order parameters*, each of which describes a *broken global symmetry*.

1.3.1 Spontaneous symmetry breaking

In quantum mechanics, the eigenstates of a Hamiltonian H_0 which commutes with all the *generators* of a symmetry group G may be classified according to the *representations* of that group. Typically this entails the appearance of degeneracies in the eigenspectrum, with degenerate states transforming into each other under the group operations. Adding a perturbation V to the Hamiltonian which breaks G down to a subgroup H will accordingly split these degeneracies, and the new multiplets of $H = H_0 + V$ are characterized by representations of the lower symmetry group H.

In quantum field theory, or in the thermodynamic limit of a classical system, as a consequence of the infinite number of degrees of freedom, symmetries may be *spontaneously broken*. This means that even if the Hamiltonian *H* (or action *S*) for the field theory is invariant under a group G of symmetry transformations, the ground state or thermodynamic density matrix may not be invariant under the full symmetry group G. The presence or absence of spontaneous symmetry breaking (SSB), and its detailed manifestations, will in general depend on the couplings, or the temperature in the case of quantum statistical mechanics. SSB is usually associated with the presence of a local *order parameter* which transforms nontrivially under some



Figure 1.4: Left: Phase diagram of H_2O in the (T, p) plane. Right: Low temperature $(T \approx 150 \text{ mK})$ longitudinal resistivity ρ_{xx} and Hall resistivity ρ_{xy} as a function of applied magnetic field in a two-dimensional electron gas system (GaAs/AlGaAs heterostructure), from R. Willett *et al.*, *Phys. Rev. Lett.* **59**, 1776 (1987). Each dip in ρ_{xx} and concomitant plateau in ρ_{xy} corresponds to a distinct phase of matter.

group operations, and whose whose quantum statistical average vanishes in a fully symmetric phase, but takes nonzero values in symmetry-broken phase¹¹. The parade example is the Ising model, $H = -\sum_{i < j} J_{ij} \sigma_i \sigma_j$, where each $\sigma_i = \pm 1$, the subscript *i* indexes a physical location in space, such as a site \mathbf{R}_i on a particular lattice. The model is explicitly \mathbb{Z}_2 symmetric under $\sigma_i \rightarrow \varepsilon \sigma_i$ for all *i*, where $\varepsilon \in \{+1, -1\}$, yet if the interaction matrix $J_{ij} = J(\mathbf{R}_i - \mathbf{R}_j)$ is short-ranged and the space dimension *d* is greater than one, there is a *critical temperature* T_c below which SSB sets in, and the system develops a spontaneous magnetization $\phi = \langle \sigma_i \rangle$. You know how in quantum mechanics, the eigenstates of a particle moving in one-dimensional double-well potential V(x) = V(-x) can be classified by their parity eigenvalues P, and the lowest two energy states are respectively symmetric (P = +1) and antisymmetric (P = -1), and are delocalized among both wells. For a quantum field theory, however, with (Euclidean) Lagrangian density $\mathcal{L}_{\rm E} = \frac{1}{2} (\nabla \phi)^2 + V(\phi)$, for d > 1 and $T < T_c$, the system actually picks the left or the right well, so that $\langle \phi(\mathbf{r}) \rangle \neq 0$. Another example is the spontaneously broken O(2) invariance of superfluids, where the boson annihilation operator $\psi(\mathbf{r})$ develops a spontaneous average $\langle \psi(\mathbf{r}) \rangle = \sqrt{n_0} e^{i\theta}$, where n_0 is the condensate density and θ the condensate phase.

Truth be told, the above description is a bit of a swindle. In the ferromagnetic $(J_{ij} > 0)$ Ising model, for example, at T = 0, there are still two ground states, $|\uparrow\rangle \equiv |\uparrow\uparrow\uparrow\cdots\rangle$ and $|\downarrow\rangle \equiv |\downarrow\downarrow\downarrow\downarrow\cdots\rangle$. The (ergodic) zero temperature density matrix is $\rho_0 = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$, and

¹¹While SSB is generally associated with the existence of a phase transitions, not all phase transitions involve SSB. Exceptions include the Kosterlitz-Thouless transition, and also those topological phases which have no local order parameter.

therefore $\langle \sigma_i \rangle = \text{Tr} (\rho_0 \sigma_i) = 0$. The order parameter apparently has vanished. WTF?! There are at least two compelling ways to resolve this seeming conundrum:

- (a) First, rather than defining the order parameter of the Ising model, for example, to be the expected value $m = \langle \sigma_i \rangle$ of the local spin¹², consider instead the behavior of the *correlation* function $C_{ij} = \langle \sigma_i \sigma_j \rangle$ in the limit $d_{ij} = |\mathbf{R}_i \mathbf{R}_j| \to \infty$. In a disordered phase, there is no correlation between infinitely far separated spins, hence $\lim_{d_{ij}\to\infty} C_{ij} = 0$. In the ordered phase, this is no longer true, and we define the *spontaneous magnetization* m from the long distance correlator: $m^2 \equiv \lim_{d_{ij}\to\infty} \langle \sigma_i \sigma_j \rangle$. In this formulatio, SSB is associated with the emergence of *long-ranged order* in the correlators of operators which transform nontrivially under the symmetry group.
- (ii) Second, we could impose an external field which *explicitly* breaks the symmetry, such as a Zeeman term $H' = -h \sum_i \sigma_i$ in the Ising model. We now compute the magnetization (per site) $m(T, h, V) = \langle \sigma_i \rangle$ as a function of temperature *T*, the external field *h*, *and* the volume *V* of our system. The order parameter m(T) in zero field is then defined as

$$m(T) = \lim_{h \to 0} \lim_{V \to \infty} m(T, h, V) \quad . \tag{1.27}$$

The order of limits here is crucially important. The thermodynamic limit $V \to \infty$ is taken first, which means that the energy difference between $|\uparrow\rangle$ and $|\downarrow\rangle$, being proportional to hV, diverges, thus infinitely suppressing the $|\downarrow\rangle$ state if h > 0 (and the $|\uparrow\rangle$ state if h < 0). The magnitude of the order parameter will be independent on the way in which we take $h \to 0$, but its sign will depend on whether $h \to 0^+$ or $h \to 0^-$, with sgn(m) = sgn(h). Physically, the direction in which a system orders can be decided by the presence of small stray fields or impurities. An illustration of how this works in the case of ideal Bose gas condensation is provided in the appendix §1.7 below.

Note that in both formulations, SSB is necessarily associated with the existence of a local operator \mathcal{O}_i which is identified as the order parameter field. In (i) the correlations $\langle \mathcal{O}_i \mathcal{O}_j \rangle$ exhibit long-ranged order in the symmetry-broken phase. In (ii) \mathcal{O}_i is the operator to which the external field h_i couples.

For a ferromagnet, the order parameter is the magnetization density, m, and the broken symmetry is the group of rotations O(3) or SU(2), or possibly \mathbb{Z}_2 . Under a group operation $g \in G$, the order parameter transforms as $m \to gm$. For a crystal or charge density wave, the order parameters are the Fourier components ϱ_G of the density at a series of wavevectors which comprise the reciprocal lattice of the structure. The broken symmetry is that of continuous translation, *i.e.* the group \mathbb{R}^d under addition, and under the group operation t_a corresponding to translation by $a \in \mathbb{R}^d$, we have $\varrho_G \to t_a \, \varrho_G = \varrho_G \, e^{iG \cdot a}$. A given order parameter ϕ will in general depend on temperature T, pressure p, applied magnetic field H, various coupling parameters which

¹²We assume translational invariance, which means $\langle \sigma_i \rangle$ is independent of the site index *i*.

enter the Hamiltonian $\{g_i\}$, *etc.* A multidimensional plot which labels the various phases of a system as a function of all these parameters is known as a *phase diagram*. Points, lines, or surfaces separating different phases are the loci of *phase transitions*, where the free energy and the order parameters of the system exhibit singularities. At a *first order transition*, certain properties change discontinuously. The canonical example of a first order transition is the freezing or boiling of liquid water to solid ice or gaseous vapor. These transitions involve a discontinuous change in the density as T or p is varied so as to cross a phase boundary¹³. At a *second order transition*, one or more order parameters vanish as a phase boundary is approached. Within the Landau paradigm, a nonzero order parameter is associated with the spontaneous breaking of a symmetry, such as spin rotation (in a magnet), space translation (in a crystal), *etc.* Furthermore, a second order transition between phases A and B is possible only if the symmetry groups G_A of the A phase and G_B of the B phase, both of which must be subgroups of the symmetry group G of the Hamiltonian, satisfy $G_A \subset G_B$ or $G_B \subset G_A$. A phase transition which takes place at T = 0 as a function of other parameters (p, H, *etc.*) is called a *quantum phase transition*.

1.3.2 Beyond the Landau paradigm

The classical O(2) model in d = 2 is precluded from achieving long-ranged order and spontaneous O(2) symmetry breaking at any finite temperature by the Hohenberg-Mermin-Wagner theorem, which we shall discuss below in $\S1.5.3$. Nevertheless, the model does exhibit a second order phase transition, known as the Berezinskii-Kosterlitz-Thouless (BKT) transition¹⁴. The energy density in the continuum model is written as $\varepsilon(\mathbf{r}) = \frac{1}{2}\rho_s(\nabla\Theta)^2$, where ρ_s is the *stiffness parameter* and $\Theta(\mathbf{r})$ is a planar angle, with Θ and $\Theta + 2\pi n$ identified for all integers n. The model features point defects which are known as vortices, about which the winding number $\oint_{C} d\mathbf{r} \cdot \nabla \Theta$ along a small loop C enclosing the vortex is $2\pi q$, where $q \in \mathbb{Z}$ is the vorticity. Integrating the energy density for a single q = 1 vortex with $\Theta(\mathbf{r}) = \tan^{-1}(y/x)$ yields $E = \pi \rho_s \ln(R/a)$, where R is the system radius and a an ultraviolet cutoff, which is naturally imposed in any lattice-based model. Since a vortex can be in any location, its entropy is $S = k_{\rm B} \ln(R^2/a^2)$, and we see that free vortices should proliferate when $F = E - TS = (\pi \rho_{\rm s} - 2k_{\rm B}T) \ln(R/a) < 0$, *i.e.* $T > T_{\rm c} = \pi \rho_{\rm s}/2k_{\rm B}$. This very crude derivation, which neglects interactions between the vortices, is essentially correct. The phase transition is associated with an *unbinding* of vortex-antivortex pairs. In the confined phase, where $T < T_c$, the correlation function $C(\mathbf{r},T) = \langle e^{i\Theta(\mathbf{r})} e^{-i\Theta(\mathbf{0})} \rangle$ decays as a power law, and there is no long-ranged order associated with a spontaneous breaking of O(2). In the plasma phase, where $T > T_c$, free vortices and antivortices (*i.e.* defects with $q_i < 0$) are present, and $C(\mathbf{r}, T)$ decays exponentially with a finite correlation length ξ . We will discuss the BKT transition and its analysis via the renormalization group later in this course.

¹³The phase boundary between liquid and vapor terminates in a *critical point*, and it is therefore possible to continuously evolve from liquid to vapor without ever encountering a singularity. Thus, from the point of view of order parameters and broken symmetry, there is no essential distinction between liquid and vapor phases.

 ¹⁴V. L. Berezinskii, Sov. Phys. JETP **32**, 493 (1971); J. M. Kosterlitz and D. J. Thouless, J. Phys. C: Solid State Phys. 6, 1181 (1973).

Over the past 25 years or so, a new paradigm has emerged for certain phases of matter which have no order parameter in the conventional sense. These are called *topological phases*, and are exemplified by the phases of the quantum Hall effect. Typically topological phases exhibit a *bulk excitation gap*, meaning it requires a finite amount of energy in order to excite these systems in their bulk, and in this respect, they are akin to insulators. However, at the edges of finite systems, there exist *gapless edge states* which may carry current. The structure of the edge states is intimately related to the nature of the bulk phase, which despite being a condensate of sorts, has no local order parameter. Topological phases are of intense current interest, both theoretically and experimentally, but they remain somewhat exotic, as compared with, say, metals. Yet the metallic phase, which is an example of a *Landau Fermi liquid*, is difficult to characterize in terms of a conventional order parameter¹⁵. Another violation of the Landau paradigm which has been revealed in recent years is the (at this point purely theoretical) notion of *deconfined quantum criticality*. A deconfined quantum critical point violated the Landau requirement that the symmetry groups on either side of the transition have a subgroup relation.

Experimental probes

We will initially study two important phases of condensed matter in the solid state: metals and insulators¹⁶. Later we shall expand our horizons and consider magnets, superconductors, quantum Hall phases, and spin liquids. These various phases are revealed through various experimental probes, including *thermodynamic measurements* such as specific heat and magnetic susceptibility, *transport measurements* such as electrical resistivity and thermal conductivity, and *spectroscopies* such as Auger, photoemission and scanning probe measurements, and *optical properties* as measured in reflectivity, Kerr effect, dichroism, *etc.* The theoretical understanding of such probes typically involves the computation of correlation (or, equivalently, response) functions within the framework of quantum statistical physics.

When falsifiable theoretical models and their solutions are in harmonious agreement with experiment, and predict new observable phenomena, we can feel confident that we are indeed beginning to understand what the world is made of.

1.4 Landau Theory of Phase Transitions

Landau's theory of phase transitions is based on an expansion of the free energy of a thermodynamic system in terms of an *order parameter*, which is nonzero in an ordered phase and zero in a disordered phase. For example, the magnetization M of a ferromagnet in zero external

¹⁵The order parameter of a Fermi liquid is usually taken to be the *quasiparticle weight* Z, which, in isotropic systems, characterizes the discontinuous drop in the momentum occupation function n(k) as one crosses the Fermi surface at $k = k_{\rm F}$.

¹⁶As we shall see, semiconductors form a sub-class of insulators.



Figure 1.5: Phase diagram for the quartic Landau free energy $f = f_0 + \frac{1}{2}am^2 + \frac{1}{4}bm^4 - hm$, with b > 0. There is a first order line at h = 0 extending from $a = -\infty$ and terminating in a critical point at a = 0. For $|h| < h^*(a)$ (dashed red line) there are three solutions to the mean field equation, corresponding to one global minimum, one local minimum, and one local maximum. Insets show behavior of the free energy f(m).

field but at finite temperature typically vanishes for temperatures $T > T_c$, where T_c is the *crit*ical temperature, also called the *Curie temperature* in a ferromagnet. A low order expansion in powers of the order parameter is appropriate sufficiently close to the phase transition, *i.e.* at temperatures such that the order parameter, if nonzero, is still small.

1.4.1 Quartic free energy with Ising symmetry

The simplest example is the quartic free energy,

$$f(m, h = 0, \theta) = f_0 + \frac{1}{2}am^2 + \frac{1}{4}bm^4 , \qquad (1.28)$$

where $f_0 = f_0(\theta)$, $a = a(\theta)$, and $b = b(\theta)$. Here, θ is a dimensionless measure of the temperature. If for example the local exchange energy in the ferromagnet is J, then we might define $\theta = k_{\rm B}T/zJ$, where z is the lattice coordination number. Let us assume b > 0, which is necessary if the free energy is to be bounded from below¹⁷. The equation of state,

$$\frac{\partial f}{\partial m} = 0 = am + bm^3 , \qquad (1.29)$$

has three solutions in the complex *m* plane: (i) m = 0, (ii) $m = \sqrt{-a/b}$, and (iii) $m = -\sqrt{-a/b}$. The latter two solutions lie along the (physical) real axis if a < 0. We assume that there exists a unique temperature θ_c where $a(\theta_c) = 0$. Minimizing *f*, we find

$$\theta < \theta_{c} \quad : \quad f(\theta) = f_{0} - \frac{a^{2}}{4b}$$

$$\theta > \theta_{c} \quad : \quad f(\theta) = f_{0} .$$

$$(1.30)$$

The free energy is continuous at θ_c since $a(\theta_c) = 0$. The specific heat, however, is discontinuous across the transition, with

$$c(\theta_{\rm c}^+) - c(\theta_{\rm c}^-) = -\theta_{\rm c} \left. \frac{\partial^2}{\partial \theta^2} \right|_{\theta = \theta_{\rm c}} \left(\frac{a^2}{4b} \right) = -\frac{\theta_{\rm c} \left[a'(\theta_{\rm c}) \right]^2}{2b(\theta_{\rm c})} \,. \tag{1.31}$$

The presence of a magnetic field *h* breaks the \mathbb{Z}_2 symmetry of $m \rightarrow -m$. The free energy becomes

$$f(m,h,\theta) = f_0 + \frac{1}{2}am^2 + \frac{1}{4}bm^4 - hm , \qquad (1.32)$$

and the mean field equation is

$$bm^3 + am - h = 0. (1.33)$$

This is a cubic equation for m with real coefficients, and as such it can either have three real solutions or one real solution and two complex solutions related by complex conjugation. Clearly we must have a < 0 in order to have three real roots, since $bm^3 + am$ is monotonically increasing otherwise. The boundary between these two classes of solution sets occurs when two roots coincide, which means f''(m) = 0 as well as f'(m) = 0. Simultaneously solving these two equations, we find

$$h^*(a) = \pm \frac{2}{3^{3/2}} \frac{(-a)^{3/2}}{b^{1/2}}, \qquad (1.34)$$

or, equivalently,

$$a^*(h) = -\frac{3}{2^{2/3}} b^{1/3} |h|^{2/3}.$$
(1.35)

If, for fixed *h*, we have $a < a^*(h)$, then there will be three real solutions to the mean field equation f'(m) = 0, one of which is a global minimum (the one for which $m \cdot h > 0$). For

¹⁷It is always the case that f is bounded from below, on physical grounds. Were b negative, we'd have to consider higher order terms in the Landau expansion.

 $a > a^*(h)$ there is only a single global minimum, at which *m* also has the same sign as *h*. If we solve the mean field equation perturbatively in h/a, we find

$$m(a,h) = \frac{h}{a} - \frac{b}{a^4} h^3 + \mathcal{O}(h^5) \qquad (a > 0)$$

$$= \pm \frac{|a|^{1/2}}{b^{1/2}} + \frac{h}{2|a|} \pm \frac{3b^{1/2}}{8|a|^{5/2}} h^2 + \mathcal{O}(h^3) \qquad (a < 0).$$
(1.36)

1.4.2 Cubic terms in Landau theory : first order transitions

Next, consider a free energy with a cubic term,

$$f = f_0 + \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4 , \qquad (1.37)$$

with b > 0 for stability. Without loss of generality, we may assume y > 0 (else send $m \to -m$). Note that we no longer have $m \to -m$ (*i.e.* \mathbb{Z}_2) symmetry. The cubic term favors positive m. What is the phase diagram in the (a, y) plane?

Extremizing the free energy with respect to m, we obtain

$$\frac{\partial f}{\partial m} = 0 = am - ym^2 + bm^3 . \tag{1.38}$$

This cubic equation factorizes into a linear and quadratic piece, and hence may be solved simply. The three solutions are m = 0 and

$$m = m_{\pm} \equiv \frac{y}{2b} \pm \sqrt{\left(\frac{y}{2b}\right)^2 - \frac{a}{b}} \,. \tag{1.39}$$

We now see that for $y^2 < 4ab$ there is only one real solution, at m = 0, while for $y^2 > 4ab$ there are three real solutions. Which solution has lowest free energy? To find out, we compare the energy f(0) with $f(m_+)^{18}$. Thus, we set

$$f(m) = f(0) \implies \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4 = 0$$
, (1.40)

and we now have two quadratic equations to solve simultaneously:

$$0 = a - ym + bm^{2}$$

$$0 = \frac{1}{2}a - \frac{1}{3}ym + \frac{1}{4}bm^{2} = 0.$$
(1.41)

Eliminating the quadratic term gives m = 3a/y. Finally, substituting $m = m_+$ gives us a relation between a, b, and y:

$$y^2 = \frac{9}{2} ab . (1.42)$$

¹⁸We needn't waste our time considering the $m = m_{-}$ solution, since the cubic term prefers positive m.



Figure 1.6: Behavior of the quartic free energy $f(m) = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$. A: $y^2 < 4ab$; B: $4ab < y^2 < \frac{9}{2}ab$; C and D: $y^2 > \frac{9}{2}ab$. The thick black line denotes a line of first order transitions, where the order parameter is discontinuous across the transition.

Thus, we have the following:

$$a > \frac{y^2}{4b} : 1 \text{ real root } m = 0$$

$$\frac{y^2}{4b} > a > \frac{2y^2}{9b} : 3 \text{ real roots; minimum at } m = 0$$

$$\frac{2y^2}{9b} > a : 3 \text{ real roots; minimum at } m = \frac{y}{2b} + \sqrt{\left(\frac{y}{2b}\right)^2 - \frac{a}{b}}$$
(1.43)

The solution m = 0 lies at a local minimum of the free energy for a > 0 and at a local maximum for a < 0. Over the range $\frac{y^2}{4b} > a > \frac{2y^2}{9b}$, then, there is a global minimum at m = 0, a local minimum at $m = m_+$, and a local maximum at $m = m_-$, with $m_+ > m_- > 0$. For $\frac{2y^2}{9b} > a > 0$, there is a local minimum at a = 0, a global minimum at $m = m_+$, and a local maximum at $m = m_-$, again with $m_+ > m_- > 0$. For a < 0, there is a local maximum at m = 0, a local minimum at $m = m_-$, and a global minimum at $m = m_+$, with $m_+ > 0 > m_-$. See fig. 1.6.

With y = 0, we have a second order transition at a = 0. With $y \neq 0$, there is a discontinuous (first order) transition at $a_c = 2y^2/9b > 0$ and $m_c = 2y/3b$. This occurs before *a* reaches the value a = 0 where the curvature at m = 0 turns negative. If we write $a = \alpha(T - T_0)$, then the expected second order transition at $T = T_0$ is *preempted* by a first order transition at $T_c = T_0 + 2y^2/9\alpha b$.

1.4.3 Magnetization dynamics

Suppose we now impose some dynamics on the system, of the simple relaxational type

$$\frac{\partial m}{\partial t} = -\Gamma \,\frac{\partial f}{\partial m}\,,\tag{1.44}$$

where Γ is a phenomenological kinetic coefficient. Assuming y > 0 and b > 0, it is convenient to adimensionalize by writing

$$m \equiv \frac{y}{b} \cdot u$$
 , $a \equiv \frac{y^2}{b} \cdot r$, $t \equiv \frac{b}{\Gamma y^2} \cdot s$. (1.45)

Then we obtain

$$\frac{\partial u}{\partial s} = -\frac{\partial \varphi}{\partial u} , \qquad (1.46)$$

where the dimensionless free energy function is

$$\varphi(u) = \frac{1}{2}ru^2 - \frac{1}{3}u^3 + \frac{1}{4}u^4 .$$
(1.47)

We see that there is a single control parameter, *r*. The fixed points of the dynamics are then the stationary points of $\varphi(u)$, where $\varphi'(u) = 0$, with

$$\varphi'(u) = u \left(r - u + u^2 \right). \tag{1.48}$$

The solutions to $\varphi'(u) = 0$ are then given by

$$u^* = 0$$
 , $u^* = \frac{1}{2} \pm \sqrt{\frac{1}{4} - r}$ (1.49)

For $r > \frac{1}{4}$ there is one fixed point at u = 0, which is attractive under the dynamics $\dot{u} = -\varphi'(u)$ since $\varphi''(0) = r$. At $r = \frac{1}{4}$ there occurs a saddle-node bifurcation and a pair of fixed points is generated, one stable and one unstable. As we see from fig. 1.5, the interior fixed point is always unstable and the two exterior fixed points are always stable. At r = 0 there is a transcritical bifurcation where two fixed points of opposite stability collide and bounce off one another (metaphorically speaking).

At the saddle-node bifurcation, $r = \frac{1}{4}$ and $u = \frac{1}{2}$, and we find $\varphi(u = \frac{1}{2}; r = \frac{1}{4}) = \frac{1}{192}$, which is positive. Thus, the thermodynamic state of the system remains at u = 0 until the value of $\varphi(u_+)$ crosses zero. This occurs when $\varphi(u) = 0$ and $\varphi'(u) = 0$, the simultaneous solution of which yields $r = \frac{2}{9}$ and $u = \frac{2}{3}$.

Suppose we slowly ramp the control parameter r up and down as a function of the dimensionless time s. Under the dynamics of eqn. 1.46, u(s) flows to the first stable fixed point encountered – this is always the case for a dynamical system with a one-dimensional phase space. Then as r is further varied, u follows the position of whatever locally stable fixed point



Figure 1.7: Fixed points for $\varphi(u) = \frac{1}{2}ru^2 - \frac{1}{3}u^3 + \frac{1}{4}u^4$ and flow under the dynamics $\dot{u} = -\varphi'(u)$. Solid curves represent stable fixed points and dashed curves unstable fixed points. Magenta arrows show behavior under slowly increasing control parameter r and dark blue arrows show behavior under slowly decreasing r. For u > 0 there is a hysteresis loop. The thick black curve shows the equilibrium thermodynamic value of u(r), *i.e.* that value which minimizes the free energy $\varphi(u)$. There is a first order phase transition at $r = \frac{2}{9}$, where the thermodynamic value of u jumps from u = 0 to $u = \frac{2}{3}$.

it initially encountered. Thus, u(r(s)) evolves smoothly until a bifurcation is encountered. The situation is depicted by the arrows in fig. 1.7. The equilibrium thermodynamic value for u(r) is discontinuous; there is a first order phase transition at $r = \frac{2}{9}$, as we've already seen. As r is increased, u(r) follows a trajectory indicated by the magenta arrows. For an negative initial value of u, the evolution as a function of r will be *reversible*. However, if u(0) is initially positive, then the system exhibits *hysteresis*, as shown. Starting with a large positive value of r, u(s) quickly evolves to $u = 0^+$, which means a positive infinitesimal value. Then as r is decreased, the system remains at $u = 0^+$ even through the first order transition, because u = 0 is an attractive fixed point. However, once r begins to go negative, the u = 0 fixed point becomes repulsive, and u(s) quickly flows to the stable fixed point $u_+ = \frac{1}{2} + \sqrt{\frac{1}{4} - r}$. Further decreasing r, the system remains on this branch. If r is later increased, then u(s) remains on the upper branch past r = 0, until the u_+ fixed point annihilates with the unstable fixed point at $u_- = \frac{1}{2} - \sqrt{\frac{1}{4} - r}$, at which time u(s) quickly flows down to $u = 0^+$ again.

1.4.4 Sixth order Landau theory : tricritical point

Finally, consider a model with \mathbb{Z}_2 symmetry, with the Landau free energy

$$f = f_0 + \frac{1}{2}am^2 + \frac{1}{4}bm^4 + \frac{1}{6}cm^6 , \qquad (1.50)$$

with c > 0 for stability. We seek the phase diagram in the (a, b) plane. Extremizing f with respect to m, we obtain

$$\frac{\partial f}{\partial m} = 0 = m \left(a + bm^2 + cm^4 \right), \qquad (1.51)$$

which is a quintic with five solutions over the complex m plane. One solution is obviously m = 0. The other four are

$$m = \pm \sqrt{-\frac{b}{2c}} \pm \sqrt{\left(\frac{b}{2c}\right)^2 - \frac{a}{c}}.$$
(1.52)

For each \pm symbol in the above equation, there are two options, hence four roots in all.

If a > 0 and b > 0, then four of the roots are imaginary and there is a unique minimum at m = 0.

For a < 0, there are only three solutions to f'(m) = 0 for real m, since the – choice for the \pm sign under the radical leads to imaginary roots. One of the solutions is m = 0. The other two are

$$m = \pm \sqrt{-\frac{b}{2c}} + \sqrt{\left(\frac{b}{2c}\right)^2 - \frac{a}{c}}.$$
(1.53)

The most interesting situation is a > 0 and b < 0. If a > 0 and $b < -2\sqrt{ac}$, all five roots are real. There must be three minima, separated by two local maxima. Clearly if m^* is a solution, then so is $-m^*$. Thus, the only question is whether the outer minima are of lower energy than the minimum at m = 0. We assess this by demanding $f(m^*) = f(0)$, where m^* is the position of the largest root (*i.e.* the rightmost minimum). This gives a second quadratic equation,

$$0 = \frac{1}{2}a + \frac{1}{4}bm^2 + \frac{1}{6}cm^4 , \qquad (1.54)$$

which together with equation 1.51 gives

$$b = -\frac{4}{\sqrt{3}}\sqrt{ac} . \tag{1.55}$$

Thus, we have the following, for fixed a > 0:

$$b > -2\sqrt{ac} : 1 \text{ real root } m = 0$$

$$-2\sqrt{ac} > b > -\frac{4}{\sqrt{3}}\sqrt{ac} : 5 \text{ real roots; minimum at } m = 0$$

$$-\frac{4}{\sqrt{3}}\sqrt{ac} > b : 5 \text{ real roots; minima at } m = \pm\sqrt{-\frac{b}{2c} + \sqrt{\left(\frac{b}{2c}\right)^2 - \frac{a}{c}}}$$
(1.56)

The point (a, b) = (0, 0), which lies at the confluence of a first order line and a second order line, is known as a *tricritical point*.



Figure 1.8: Behavior of the sextic free energy $f(m) = \frac{1}{2}am^2 + \frac{1}{4}bm^4 + \frac{1}{6}cm^6$. A: a > 0 and b > 0; B: a < 0 and b > 0; C: a < 0 and b < 0; D: a > 0 and $b < -\frac{4}{\sqrt{3}}\sqrt{ac}$; E: a > 0 and $-\frac{4}{\sqrt{3}}\sqrt{ac}$; E: a > 0 and $-\frac{4}{\sqrt{3}}\sqrt{ac}$; E: a > 0 and $-\frac{4}{\sqrt{3}}\sqrt{ac}$; E: a > 0 and $-2\sqrt{ac} < b < 0$. The thick dashed line is a line of second order transitions, which meets the thick solid line of first order transitions at the tricritical point, (a, b) = (0, 0).

The case of barium titanate

The compound $BaTiO_3$ is a *ferroelectric* in which, at sufficiently low temperatures, a spontaneous electric polarization density *P* develops. The Landau free energy density may be written as

$$f(P,\varepsilon) = f_0 + \frac{1}{2}aP^2 + \frac{1}{4}bP^4 + \frac{1}{6}cP^6 - dEP + \varepsilon P^2 + \frac{\varepsilon^2}{2k} \quad , \tag{1.57}$$

where *E* is the electric field and ε is a component of the the strain field¹⁹. Note that the coupling between strain and polarization is linear in the former and quadratic in the latter, which is a

¹⁹Recall the strain tensor in a solid is given by $\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x^j} + \frac{\partial u_j}{\partial x^i} \right)$, where $\boldsymbol{u}(\boldsymbol{r})$ is the local displacement field.



Figure 1.9: High temperature cubic perovskite crystal structure of $BaTiO_3$. Ba^{2+} sites are in green, Ti^{4+} in blue, and O^{2-} in red. The yellow arrow shows the direction in which the Ti^{4+} ion moves as the material is cooled below T_c within the displacive model. Image credit: Wikipedia.

consequence of symmetry associated with the displacive transition. In other materials such as KH_2PO_4 , where the symmetry is lower, the coupling is of the form εP .

Setting $\partial f/\partial \varepsilon = 0$ we obtain $\varepsilon = -kdP^2$, resulting in the the effective free energy density

$$f_{\text{eff}}(P) = f_0 + \frac{1}{2}aP^2 + (\frac{1}{4}b - \frac{1}{2}kd^2)P^4 + \frac{1}{6}cP^6 - EP \quad . \tag{1.58}$$

If b > 0, and $dk^2 > \frac{1}{2}b$, the second order transition is driven to become first order due to the coupling to strain. However, it is oftentimes possible under experimental conditions to ensure that the strain is always zero, for example in the case of a thin epitaxial film whose lattice constants are perfectly matched to a substrate. In this case, stresses develop which constrain the strain to be $\varepsilon = 0$, and in the absence of an electric field *E* the transition is second order.

1.4.5 Hysteresis for the sextic potential

Once again, we consider the dissipative dynamics $\dot{m} = -\Gamma f'(m)$. We adimensionalize by writing

$$m \equiv \sqrt{\frac{|b|}{c}} \cdot u \quad , \quad a \equiv \frac{b^2}{c} \cdot r \quad , \quad t \equiv \frac{c}{\Gamma b^2} \cdot s .$$
 (1.59)

Then we obtain once again the dimensionless equation

$$\frac{\partial u}{\partial s} = -\frac{\partial \varphi}{\partial u} , \qquad (1.60)$$



Figure 1.10: Free energy $\varphi(u) = \frac{1}{2}ru^2 - \frac{1}{4}u^4 + \frac{1}{6}u^6$ for several different values of the control parameter r.

where

$$\varphi(u) = \frac{1}{2}ru^2 \pm \frac{1}{4}u^4 + \frac{1}{6}u^6 . \tag{1.61}$$

In the above equation, the coefficient of the quartic term is positive if b > 0 and negative if b < 0. That is, the coefficient is sgn(b). When b > 0 we can ignore the sextic term for sufficiently small u, and we recover the quartic free energy studied earlier. There is then a second order transition at r = 0.

New and interesting behavior occurs for b > 0. The fixed points of the dynamics are obtained by setting $\varphi'(u) = 0$. We have

$$\varphi(u) = \frac{1}{2}ru^2 - \frac{1}{4}u^4 + \frac{1}{6}u^6$$

$$\varphi'(u) = u\left(r - u^2 + u^4\right).$$
(1.62)

Thus, the equation $\varphi'(u) = 0$ factorizes into a linear factor u and a quartic factor $u^4 - u^2 + r$ which is quadratic in u^2 . Thus, we can easily obtain the roots:

$$r < 0 \quad : \quad u^* = 0 , \ u^* = \pm \sqrt{\frac{1}{2} + \sqrt{\frac{1}{4} - r}}$$

$$0 < r < \frac{1}{4} \quad : \quad u^* = 0 , \ u^* = \pm \sqrt{\frac{1}{2} + \sqrt{\frac{1}{4} - r}} , \ u^* = \pm \sqrt{\frac{1}{2} - \sqrt{\frac{1}{4} - r}}$$

$$r > \frac{1}{4} \quad : \quad u^* = 0 .$$
(1.63)



Figure 1.11: Fixed points $\varphi'(u^*) = 0$ for the sextic potential $\varphi(u) = \frac{1}{2}ru^2 - \frac{1}{4}u^4 + \frac{1}{6}u^6$, and corresponding dynamical flow (arrows) under $\dot{u} = -\varphi'(u)$. Solid curves show stable fixed points and dashed curves show unstable fixed points. The thick solid black and solid grey curves indicate the equilibrium thermodynamic values for u; note the overall $u \to -u$ symmetry. Within the region $r \in [0, \frac{1}{4}]$ the dynamics are irreversible and the system exhibits the phenomenon of hysteresis. There is a first order phase transition at $r = \frac{3}{16}$.

In fig. 1.11, we plot the fixed points and the hysteresis loops for this system. At $r = \frac{1}{4}$, there are two symmetrically located saddle-node bifurcations at $u = \pm \frac{1}{\sqrt{2}}$. We find $\varphi(u = \pm \frac{1}{\sqrt{2}}, r = \frac{1}{4}) = \frac{1}{48}$, which is positive, indicating that the stable fixed point $u^* = 0$ remains the thermodynamic minimum for the free energy $\varphi(u)$ as r is decreased through $r = \frac{1}{4}$. Setting $\varphi(u) = 0$ and $\varphi'(u) = 0$ simultaneously, we obtain $r = \frac{3}{16}$ and $u = \pm \frac{\sqrt{3}}{2}$. The thermodynamic value for u therefore jumps discontinuously from u = 0 to $u = \pm \frac{\sqrt{3}}{2}$ (either branch) at $r = \frac{3}{16}$; this is a first order transition.

Under the dissipative dynamics considered here, the system exhibits hysteresis, as indicated in the figure, where the arrows show the evolution of u(s) for very slowly varying r(s). When the control parameter r is large and positive, the flow is toward the sole fixed point at $u^* = 0$. At $r = \frac{1}{4}$, two simultaneous saddle-node bifurcations take place at $u^* = \pm \frac{1}{\sqrt{2}}$; the outer branch is stable and the inner branch unstable in both cases. At r = 0 there is a subcritical pitchfork bifurcation, and the fixed point at $u^* = 0$ becomes unstable.

Suppose one starts off with $r \gg \frac{1}{4}$ with some value u > 0. The flow $\dot{u} = -\varphi'(u)$ then rapidly results in $u \to 0^+$. This is the 'high temperature phase' in which there is no magnetization. Now let *r* increase slowly, using *s* as the dimensionless time variable. The scaled magnetization

 $u(s) = u^*(r(s))$ will remain pinned at the fixed point $u^* = 0^+$. As r passes through $r = \frac{1}{4}$, two new stable values of u^* appear, but our system remains at $u = 0^+$, since $u^* = 0$ is a stable fixed point. But after the subcritical pitchfork, $u^* = 0$ becomes unstable. The magnetization u(s) then flows rapidly to the stable fixed point at $u^* = \frac{1}{\sqrt{2}}$, and follows the curve $u^*(r) = (\frac{1}{2} + (\frac{1}{4} - r)^{1/2})^{1/2}$ for all r < 0.

Now suppose we start increasing r (*i.e.* increasing temperature). The magnetization follows the stable fixed point $u^*(r) = \left(\frac{1}{2} + \left(\frac{1}{4} - r\right)^{1/2}\right)^{1/2}$ past r = 0, beyond the first order phase transition point at $r = \frac{3}{16}$, and all the way up to $r = \frac{1}{4}$, at which point this fixed point is annihilated at a saddle-node bifurcation. The flow then rapidly takes $u \to u^* = 0^+$, where it remains as r continues to be increased further.

Within the region $r \in [0, \frac{1}{4}]$ of control parameter space, the dynamics are said to be *irreversible* and the behavior of u(s) is said to be *hysteretic*.

1.4.6 Weak crystallization

That *weak crystallization*, meaning crystallization in a weakly first-order transition, should result in a triangular lattice in d = 2 was argued by Alexander and McTague²⁰ based on a Landau theory of the transition. The argument is as follows. Let ρ_G be the amplitude of the Fourier component of the density $\rho(\mathbf{r})$ with wavevector \mathbf{G} , which is a reciprocal lattice vector of the incipient crystalline phase. Then construct the free energy

$$F[\{\varrho_{G}\}] = \frac{1}{2} \sum_{G} \chi^{-1}(G) |\varrho_{G}|^{2} - \frac{1}{3} B \sum_{G_{1}} \sum_{G_{2}} \sum_{G_{3}} \varrho_{G_{1}} \varrho_{G_{2}} \varrho_{G_{3}} \delta_{G_{1}+G_{2}+G_{3},0} + \frac{1}{4} C \sum_{G_{1}} \sum_{G_{2}} \sum_{G_{3}} \sum_{G_{4}} \varrho_{G_{1}} \varrho_{G_{2}} \varrho_{G_{3}} \varrho_{G_{4}} \delta_{G_{1}+G_{2}+G_{3}+G_{4},0} + \dots ,$$
(1.64)

where

$$\chi^{-1}(\mathbf{k}) = r + b \, (\mathbf{k}^2 - G^2)^2 \tag{1.65}$$

is the inverse static susceptibility at wavevector k, which for fixed r is minimized for |k| = G. The quadratic term determines the magnitude of the preferred wavevectors at which condensation takes place at $r = r_c = 0$, but this energy is degenerate over the circle (or sphere in d = 3) of radius G. For weak crystallization, then, the cubic term determines the crystal structure, and evidently prefers structures whose reciprocal lattices contain the maximum number of triangles, in order to satisfy the $G_1 + G_2 + G_3 = 0$ condition. In d = 2 this prefers a reciprocal lattice which is triangular, hence the underlying direct Bravais lattice is also triangular (or honeycomb). In d = 3, this condition prefers the fcc structure among all regular lattices, and the

²⁰S. Alexander and J. McTague, *Phys. Rev. Lett.* **41**, 702 (1978). See also E. I. Kats, V. V. Lebedev, and A. R. Muranov, *Phys. Rep.* **228**, 1 (1993).

corresponding direct lattice is thus bcc. It should be emphasized that the Alexander-McTague theory applies to the weak crystallization of a fluid, and really describes the formation of a charge density wave structure, rather than a Wigner crystal of point particles.

1.5 Four Vignettes

1.5.1 Lower critical dimension

Depending on whether the global symmetry group of a model is discrete or continuous, there exists a *lower critical dimension* d_{ℓ} at or below which no phase transition may take place at finite temperature. That is, for $d \leq d_{\ell}$, the critical temperature is $T_c = 0$. Owing to its neglect of fluctuations, mean field theory generally *overestimates* the value of T_c because it overestimates the stability of the ordered phase²¹. Indeed, there are many examples where mean field theory predicts a finite T_c when the actual critical temperature is $T_c = 0$. This happens for $d \leq d_{\ell}$.

Let's test the stability of the ordered (ferromagnetic) state of the one-dimensional Ising model at low temperatures. We consider order-destroying *domain wall* excitations which interpolate between regions of degenerate, symmetry-related ordered phase, *i.e.* $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$ and $\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$. For a system with a discrete symmetry at low temperatures, the domain wall is abrupt, on the scale of a single lattice spacing. If the exchange energy is *J*, then the energy of a single domain wall is 2J, since a link of energy -J is replaced with one of energy +J. However, there are *N* possible locations for the domain wall, hence its entropy is $k_{\rm B} \ln N$. For a system with *M* domain walls, the free energy is

$$F = 2MJ - k_{\rm B}T \ln \binom{N}{M}$$

$$= N \cdot \left\{ 2Jx + k_{\rm B}T \left[x \ln x + (1-x) \ln(1-x) \right] \right\},$$
(1.66)

²¹One can concoct models for which the mean field transition temperature *underestimates* the actual critical temperature. Consider for example an Ising model with interaction $u(\sigma, \sigma') = -\epsilon^{-1} \ln(1 + \epsilon \sigma \sigma')$, where the spins take values $\sigma, \sigma' = \pm 1$, and where $0 < \epsilon < 1$. If we write $\sigma = \langle \sigma \rangle + \delta \sigma$ at each site and neglect terms quadratic in fluctuations, the resulting mean field Hamiltonian is equivalent to a set of decoupled spins in an external field $h = zm/(1 + \epsilon m^2)$, where $m = \langle \sigma \rangle$. From the mean field equation $m = \tanh(h/T)$, one obtains the MF transition temperature is $T_c^{\rm MF} = z$, the lattice coordination number, independent of ϵ . On the other hand, we may also write $u(\sigma, \sigma') = u_{\epsilon} - J_{\epsilon} \sigma \sigma'$, where $u_{\epsilon} = -\ln(1 - \epsilon^2)/2\epsilon$ and $J_{\epsilon} = \epsilon^{-1} \tanh^{-1}(\epsilon)$. On the square lattice, where z = 4, one has the exact result $T_c(\epsilon) = 2J_{\epsilon}/\sinh^{-1}(1) = 2.269 J_{\epsilon}$, which diverges as $\epsilon \to 1$, while $T_c^{\rm MF} = 4$ remains finite. For $\epsilon > 0.9265$, one has $T_c(\epsilon) > T_c^{\rm MF}$. Finally, if instead of deriving the MFT via the 'neglect of fluctuations' method one uses a local variational density matrix of the form $\varrho = \prod_i \left[\frac{1}{2}(1 + m_i) \delta_{\sigma_i, +1} + \frac{1}{2}(1 - m_i) \delta_{\sigma_i, -1} \right]$, with m as a variational parameter, from the variational free energy density $f = N^{-1} \left[\operatorname{Tr}(\varrho H) + T \operatorname{Tr}(\varrho \ln \varrho) \right]$, one obtains the MF equation $zJ_{\epsilon}m = T \tanh^{-1}(m)$, whence $T_c^{\rm MF} = zJ_{\epsilon}$ which *does* exceed the exact result on the square lattice. So in this example, it depends on the method employed to derive the MF Hamiltonian.



Figure 1.12: Domain walls in the two-dimensional (left) and three-dimensional (right) Ising model.

where x = M/N is the density of domain walls, and where we have used Stirling's approximation for k! when k is large. Extremizing with respect to x, we find

$$\frac{x}{1-x} = e^{-2J/k_{\rm B}T} \implies x = \frac{1}{e^{2J/k_{\rm B}T} + 1}$$
 (1.67)

The average distance between domain walls is x^{-1} , which is finite for finite *T*. Thus, the thermodynamic state of the system is *disordered*, with no net average magnetization.

Consider next an Ising domain wall in *d* dimensions. Let the linear dimension of the system be $L \cdot a$, where *L* is a real number and *a* is the lattice constant. Then the energy of a single domain wall which partitions the entire system is $2J \cdot L^{d-1}$. The domain wall entropy is difficult to compute, because the wall can fluctuate significantly, but for a single domain wall we have $S \gtrsim k_{\rm B} \ln L$. Thus, the free energy $F = 2JL^{d-1} - k_{\rm B}T \ln L$ is dominated by the energy term if d > 1, suggesting that the system *may* be ordered. We can do a slightly better job in d = 2 by writing

$$Z \approx \exp\left(L^d \sum_P N_P \, e^{-2PJ/k_{\rm B}T}\right)\,,\tag{1.68}$$

where the sum is over all closd loops of perimeter P, and N_P is the number of such loops. An example of such a loop circumscribing a domain is depicted in the left panel of fig. 1.12. It turns out that

$$N_P \simeq \kappa^P P^{-\theta} \cdot \left\{ 1 + \mathcal{O}(P^{-1}) \right\}, \qquad (1.69)$$

where $\kappa = z - 1$ with z the lattice coordination number, and θ is some exponent. We can understand the κ^P factor in the following way. At each step along the perimeter of the loop, there are $\kappa = z - 1$ possible directions to go (since one doesn't backtrack). The fact that the loop must avoid overlapping itself and must return to its original position to be closed leads to the power law term $P^{-\theta}$, which is subleading since $\kappa^P P^{-\theta} = \exp(P \ln \kappa - \theta \ln P)$ and $P \gg \ln P$ for $P \gg 1$. Thus,

$$F \approx -\frac{1}{\beta} L^d \sum_P P^{-\theta} e^{(\ln \kappa - 2\beta J)P} , \qquad (1.70)$$

which diverges if $\ln \kappa > 2\beta J$, *i.e.* if $T > 2J/k_{\rm B} \ln(z-1)$. We identify this singularity with the phase transition. The high temperature phase involves a proliferation of such loops. The excluded volume effects between the loops, which we have not taken into account, then enter in an essential way so that the sum converges. Thus, we have the following picture:

 $\ln \kappa < 2\beta J$: large loops suppressed ; ordered phase $\ln \kappa > 2\beta J$: large loops proliferate ; disordered phase .

On the square lattice, we obtain

$$k_{\rm B}T_{\rm c}^{\rm approx} = \frac{2J}{\ln 3} = 1.82 J$$

 $k_{\rm B}T_{\rm c}^{\rm exact} = \frac{2J}{\sinh^{-1}(1)} = 2.27 J$

The agreement is better than we should reasonably expect from such a crude argument.

Nota bene : Beware of arguments which allegedly prove the existence of an ordered phase. Generally speaking, any approximation will *underestimate* the entropy, and thus will overestimate the stability of the putative ordered phase.

Continuous symmetries

When the global symmetry group is continuous, the domain walls interpolate smoothly between ordered phases. Consider the classical continuum O(N) model

$$H = \frac{1}{2}\rho_{\rm s} \int d^d r \, (\partial_\mu n^a)^2 \,, \tag{1.71}$$

where $\hat{n}(x) = (n^1, \dots, n^N)$ with $\hat{n}^2 = 1$. The quantity ρ_s is called the *stiffness parameter* and has dimensions of $[\rho_s] = \mathsf{EL}^{2-d}$. Any ground state configuration, such as $\hat{n}(x) = \hat{\mathbf{e}}_1$, breaks the $\mathsf{O}(N)$ symmetry.

Consider now a domain wall configuration

$$\hat{\boldsymbol{n}}(\boldsymbol{x}) = \cos(\theta(\boldsymbol{x})) \,\hat{\boldsymbol{e}}_1 + \sin(\theta(\boldsymbol{x})) \,\hat{\boldsymbol{e}}_2 \quad , \tag{1.72}$$

where $\theta(\mathbf{x}) = 2\pi q x^1/L$, which describes a slow *q*-fold ($q \in \mathbb{Z}$) twist of the unit vector $\hat{\mathbf{n}}(\mathbf{x})$ in the $(\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2)$ plane with period *L*, which we take to be the linear dimension of the sample²². The domain wall then resembles the sketch in Fig. 1.13, and its energy is computed to be

$$E = \frac{1}{2}\rho_{\rm s} L^{d-1} \int_{0}^{L} dx^{1} \left(\frac{2\pi q}{L}\right)^{2} = 2\pi^{2} q^{2} \rho_{\rm s} L^{d-2} .$$
(1.73)

²²Periodic boundary conditions are presumed.



Figure 1.13: A domain wall in an *XY* ferromagnet.

Recall that in the case of discrete symmetry, the domain wall energy scaled as $E \propto L^{d-1}$. Thus, with $S \gtrsim k_{\rm B} \ln L$ for a single wall, we see that the entropy term dominates if $d \leq 2$, in which case there is no finite temperature phase transition. Thus, the lower critical dimension d_{ℓ} depends on whether the global symmetry is discrete or continuous, with

 $\begin{array}{rcl} \mbox{discrete global symmetry} & \Longrightarrow & d_\ell = 1 \\ \mbox{continuous global symmetry} & \Longrightarrow & d_\ell = 2 \,. \end{array}$

Note that all along we have assumed local, *short-ranged* interactions. Long-ranged interactions can enhance order and thereby suppress d_{ℓ} .

Thus, we expect that for models with discrete symmetries, $d_{\ell} = 1$ and there is no finite temperature phase transition for $d \leq 1$. For models with continuous symmetries, $d_{\ell} = 2$, and we expect $T_c = 0$ for $d \leq 2$. In this context we should emphasize that the two-dimensional *XY* model *does* exhibit a phase transition at finite temperature, called the *Kosterlitz-Thouless* transition. However, this phase transition is *not* associated with the breaking of the continuous global O(2) symmetry and rather has to do with the unbinding of vortices and antivortices. So there is still no true long-ranged order below the critical temperature $T_{\rm KT}$, even though there is a phase transition!

1.5.2 Random systems : Imry-Ma argument

In condensed matter systems, intrinsic randomness often exists due to quenched impurities, grain boundaries, immobile vacancies, *etc.* How does this quenched randomness affect a system's attempt to order at T = 0? This question was taken up in a beautiful and brief paper by J. Imry and S.-K. Ma, *Phys. Rev. Lett.* **35**, 1399 (1975). Imry and Ma considered models in which there are short-ranged interactions and a random local field coupling to the local order



Figure 1.14: Left panel : Imry-Ma domains for an O(2) model. The arrows point in the direction of the local order parameter field $\langle \hat{n}(r) \rangle$. Right panel : free energy density as a function of domain size L_d . Keep in mind that the minimum possible value for L_d is the lattice spacing *a*.

parameter:

$$H_{\rm RFI} = -J \sum_{\langle ij \rangle} \sigma_i \, \sigma_j - \sum_i h_i \, \sigma_i \tag{1.74}$$

$$H_{\rm RFO(n)} = -J \sum_{\langle ij \rangle} \hat{\boldsymbol{n}}_i \cdot \hat{\boldsymbol{n}}_j - \sum_i h_i^{\alpha} n_i^{\alpha} , \qquad (1.75)$$

where

$$\langle\!\langle h_i^{\alpha} \rangle\!\rangle = 0 \qquad , \qquad \langle\!\langle h_i^{\alpha} h_j^{\beta} \rangle\!\rangle = \Gamma \,\delta^{\alpha\beta} \,\delta_{ij} \,,$$
 (1.76)

where $\langle\!\langle \cdot \rangle\!\rangle$ denotes a configurational average over the disorder. Imry and Ma reasoned that a system could try to lower its free energy by forming *domains* in which the order parameter takes advantage of local fluctuations in the random field. The size of these domains is assumed to be L_d , a length scale to be determined. See the sketch in the left panel of fig. 1.14.

There are two contributions to the energy of a given domain: bulk and surface terms. The bulk energy is

$$E_{\rm bulk} = -h_{\rm rms} \left(L_{\rm d}/a \right)^{d/2},$$
 (1.77)

where *a* is the lattice spacing. This is because when we add together $(L_d/a)^d$ random fields, the magnitude of the result is proportional to the square root of the number of terms, *i.e.* to $(L_d/a)^{d/2}$. The quantity $h_{\rm rms} = \sqrt{T}$ is the root-mean-square fluctuation in the random field at a given site. The surface energy is

$$E_{\rm surface} \propto \begin{cases} J \, (L_{\rm d}/a)^{d-1} & \text{(discrete symmetry)} \\ J \, (L_{\rm d}/a)^{d-2} & \text{(continuous symmetry)} . \end{cases}$$
(1.78)

We compute the critical dimension d_c by balancing the bulk and surface energies,

$$d-1 = \frac{1}{2}d \implies d_{c} = 2 \quad \text{(discrete)}$$

$$d-2 = \frac{1}{2}d \implies d_{c} = 4 \quad \text{(continuous)}$$

The total free energy is $F = (V/L_d^d) \cdot \Delta E$, where $\Delta E = E_{\text{bulk}} + E_{\text{surf}}$. Thus, the free energy per unit cell is

$$f = \frac{F}{V/a^d} \approx J \left(\frac{a}{L_d}\right)^{\frac{1}{2}d_c} - h_{\rm rms} \left(\frac{a}{L_d}\right)^{\frac{1}{2}d}.$$
(1.79)

If $d < d_{c'}$ the surface term dominates for small L_d and the bulk term dominates for large L_d . There is global minimum at

$$\frac{L_{\rm d}}{a} = \left(\frac{d_{\rm c}}{d} \cdot \frac{J}{h_{\rm rms}}\right)^{\frac{2}{d_{\rm c}-d}}.$$
(1.80)

For $d > d_c$, the relative dominance of the bulk and surface terms is reversed, and there is a global maximum at this value of L_d .

Sketches of the free energy $f(L_d)$ in both cases are provided in the right panel of fig. 1.14. We must keep in mind that the domain size L_d cannot become smaller than the lattice spacing a. Hence we should draw a vertical line on the graph at $L_d = a$ and discard the portion $L_d < a$ as unphysical. For $d < d_c$, we see that the state with $L_d = \infty$, *i.e.* the ordered state, is never the state of lowest free energy. In dimensions $d < d_c$, the ordered state is always unstable to domain formation in the presence of a random field.

For $d > d_c$, there are two possibilities, depending on the relative size of J and $h_{\rm rms}$. We can see this by evaluating $f(L_d = a) = J - h_{\rm rms}$ and $f(L_d = \infty) = 0$. Thus, if $J > h_{\rm rms}$, the minimum energy state occurs for $L_d = \infty$. In this case, the system has an ordered ground state, and we expect a finite temperature transition to a disordered state at some critical temperature $T_c > 0$. If, on the other hand, $J < h_{\rm rms}$, then the fluctuations in h overwhelm the exchange energy at T = 0, and the ground state is disordered down to the very smallest length scale (*i.e.* the lattice spacing a).

Please read the essay, Memories of Shang-Keng Ma.

1.5.3 Hohenberg-Mermin-Wagner theorem

The Hohenberg-Mermin-Wagner (HMW) theorem is a powerful result which establishes the absence of broken continuous symmetry for systems at any finite temperature in dimensions $d \leq 2$. Extensions of the theorem have been applied to certain d = 1 quantum systems at T = 0, such as antiferromagnets, crystals, and Bose superfluids. As we shall see, it is related to Goldstone's theorem, which we shall discuss below in §1.5.4.

Before getting into the details, a plea for proper attribution. Historically, the HMW theorem has often been referred to as the "Mermin-Wagner theorem", but in fact it should rightly be

called the "Hohenberg-Mermin-Wagner theorem"²³. For a latter day perspective, including a brief recounting of the history, see B. I. Halperin, *J. Stat. Phys.* **175**, 521 (2019).

For a poor man's derivation of the HMW theorem, we proffer the following argument. Expanding in quadratic fluctuations for a translationally invariant quantum system in the thermodynamic limit, consider the model Hamiltonian

$$H = \sum_{k} \left\{ \underbrace{\frac{p_{k} p_{-k}}{2m_{k}} + \frac{1}{2} m_{k} \omega_{k}^{2} x_{k} x_{-k}}_{k} \right\} = \sum_{k} (a_{k}^{\dagger} a_{k} + \frac{1}{2}) \hbar \omega_{k} \quad , \qquad (1.81)$$

where $[p_k, x_{k'}] = -i\hbar \delta_{k+k',0}$ and $[a_k, a_{k'}^{\dagger}] = \delta_{k,k'}$. The average energy per k mode is given by $\langle H_k \rangle = (n_k + \frac{1}{2})\hbar \omega_k$, with $n_k = 1/(\exp(\beta \hbar \omega_k) - 1)$ the mode occupancy. Now let's compute the fluctuations in the local coordinate x_r :

$$\langle x_{\mathbf{r}}^2 \rangle = \frac{1}{N} \sum_{\mathbf{k}} \langle x_{\mathbf{k}} x_{-\mathbf{k}} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \frac{(n_{\mathbf{k}} + \frac{1}{2})\hbar\omega_{\mathbf{k}}}{m_{\mathbf{k}}\omega_{\mathbf{k}}^2} = \operatorname{vol}(\Omega) \int_{\hat{\Omega}} \frac{d^d k}{(2\pi)^2} \left(\frac{1}{\exp(\beta\hbar\omega_{\mathbf{k}}) - 1} + \frac{1}{2} \right) \frac{\hbar}{m_{\mathbf{k}}\omega_{\mathbf{k}}} \quad ,$$

$$(1.82)$$

where *N* is the number of unit cells in the system, Ω is the unit cell, and $\hat{\Omega}$ is the Brillouin zone.

We presume the dispersion ω_k behaves as $\omega_k = c|\mathbf{k}|$ as $\mathbf{k} \to \mathbf{0}$, and further assume that $m_{\mathbf{k}\to 0}$ is finite. At finite temperature, the integrand therefore diverges as $T/\omega_k^2 \sim T/\mathbf{k}^2$ as $\mathbf{k} \to \mathbf{0}$, and thus the integral is IR-divergent for $d \leq 2$. This means that we have *expanded about the wrong vacuum*. Note that the same considerations apply at T = 0 in d = 1, where $n_k = 0$, due to the intrinsic quantum fluctuations.

Formal proof of the HMW theorem

We follow here the original Mermin-Wagner treatment of the HMW theorem. Consider the Heisenberg model,

$$H = -\sum_{\boldsymbol{R},\boldsymbol{R}'} J(\boldsymbol{R} - \boldsymbol{R}') \, \boldsymbol{S}_{\boldsymbol{R}} \cdot \boldsymbol{S}_{\boldsymbol{R}'} - \sum_{\boldsymbol{R}} h_{\boldsymbol{R}} \, \boldsymbol{S}_{\boldsymbol{R}}^{z} \quad . \tag{1.83}$$

Here the positions $\{R\}$ are sites on some Bravais lattice, the spin operators obey the SU(2) algebra²⁴

$$\left[S_{\boldsymbol{R}}^{\alpha}, S_{\boldsymbol{R}'}^{\beta}\right] = i\,\delta_{\boldsymbol{R}\boldsymbol{R}'}\,\epsilon^{\alpha\beta\gamma}\,S_{\boldsymbol{R}}^{\gamma} \quad , \tag{1.84}$$

and the coupling $J(\mathbf{R} - \mathbf{R}') = J(\mathbf{R}' - \mathbf{R})$ is inversion symmetric, and satisfies $J(\mathbf{0}) = 0$. The Fourier components \hat{h}_k of the magnetic field satisfy $\hat{h}_{-k} = \hat{h}_k^*$, since the Hamiltonian must be

²³P. C. Hohenberg, *Phys. Rev.* **158**, 383 (1967); N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**, 1133 (1966). ²⁴We set $\hbar = 1$ for convenience.

Hermitian. We will also need to require that the interaction kernel $J(\mathbf{R} - \mathbf{R}')$ be sufficiently short-ranged, decaying faster than $|\mathbf{R} - \mathbf{R}'|^{-(d+2)}$, as shall become clear below.

The proof proceeds by finding a bound for the magnitude $|\hat{m}_{k}|$, where $\hat{m}_{k}\equiv \langle S_{k}^{z}\rangle/N$, with

$$S_{\boldsymbol{k}}^{z} = \sum_{\boldsymbol{R}} S_{\boldsymbol{R}}^{z} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \quad . \tag{1.85}$$

The quantity m_k is the order parameter at wavevector k. For example, at k = 0 we have $\hat{m}_0 = N^{-1} \sum_{\mathbf{R}} \langle S_{\mathbf{R}}^z \rangle$, which is the moment per site. The goal is to show that in the limit $\hat{h}_k \to 0$ of vanishing external field that the order parameter must vanish if the spatial dimension d is sufficiently small.

Bogoliubov's inequality

The proof utilizes the Bogoliubov inequality,

$$\left|\left\langle [A,C]\right\rangle\right|^2 \leqslant \frac{1}{2}\beta\left\langle \{A,A^{\dagger}\}\right\rangle\left\langle \left[C^{\dagger},[H,C]\right]\right\rangle \quad,\tag{1.86}$$

for any operators *A* and *C*, where $\langle \mathcal{O} \rangle = \text{Tr} \left(\mathcal{O} e^{-\beta H} \right) / \text{Tr} e^{-\beta H}$ is the thermodynamic expectation value of the operator \mathcal{O} . To prove Eqn. 1.86, we start by defining the operator scalar product,

$$(A,B) \equiv \sum_{m \neq n} \langle n | A^{\dagger} | m \rangle \langle m | B | n \rangle \left(\frac{W_m - W_n}{E_n - E_m} \right) \quad , \tag{1.87}$$

where $W_m = e^{-\beta E_m} / \operatorname{Tr} e^{-\beta H}$ is the Boltzmann weight for the state $|m\rangle$. One can check that (\bullet, \bullet) satisfies (i) $(A, B) = (B, A)^*$ (conjugation symmetry), (ii) $(A, \lambda_1 B_1 + \lambda_2 B_2) = \lambda_1(A, B_1) + \lambda_2(A, B_2)$ (linearity), and (iii) $(A, A) \ge 0$ (positive semidefiniteness). Under these conditions, the Schwarz inequality,

$$|(A,B)|^2 \leq (A,A)(B,B)$$
, (1.88)

holds.

Let's evaluate the Schwarz inequality with $B = [C^{\dagger}, H]$. We have

$$(A, B) = (A, [C^{\dagger}, H]) = \sum_{m \neq n} \langle n | A^{\dagger} | m \rangle \langle m | (C^{\dagger}H - HC^{\dagger}) | n \rangle \left(\frac{W_m - W_n}{E_n - E_m}\right)$$

$$= \sum_{m,n} \langle n | A^{\dagger} | m \rangle \langle m | C^{\dagger} | n \rangle (W_m - W_n) = \langle [C^{\dagger}, A^{\dagger}] \rangle \quad .$$
(1.89)

Substituting A = B in this result, we have

$$(B,B) = \left\langle [C^{\dagger}, B^{\dagger}] \right\rangle = \left\langle \left[C^{\dagger}, [H, C]\right] \right\rangle \quad , \tag{1.90}$$

and thus the Schwarz inequality guarantees

$$\left|\left\langle \left[C^{\dagger}, A^{\dagger}\right]\right\rangle\right|^{2} = \left|\left\langle \left[A, C\right]\right\rangle\right|^{2} \leqslant (A, A) \left\langle \left[C^{\dagger}, \left[H, C\right]\right]\right\rangle \quad .$$

$$(1.91)$$

Next, note that

$$\frac{W_m - W_n}{E_n - E_m} = \left(\frac{W_m + W_n}{E_n - E_m}\right) \left(\frac{W_m - W_n}{W_m + W_n}\right) \\
= \left(\frac{W_m + W_n}{E_n - E_m}\right) \tanh\left(\frac{1}{2}\beta(E_n - E_m)\right) \leqslant \frac{\beta}{2} \left(W_m + W_n\right) \quad ,$$
(1.92)

since $0 \le x^{-1} \tanh x \le 1$. Thus we have

$$(A,A) \leqslant \frac{\beta}{2} \sum_{m \neq n} \langle n | A^{\dagger} | m \rangle \langle m | A | n \rangle (W_m + W_n) \leqslant \frac{\beta}{2} \langle \{A, A^{\dagger}\} \rangle \quad , \tag{1.93}$$

thereby establishing the Bogoliubov inequality of Eqn. 1.86.

Application to quantum Heisenberg model

Consider now the quantum Heisenberg model of Eqn. 1.83. Define the Fourier variables

$$S_{\boldsymbol{k}}^{\alpha} = \sum_{\boldsymbol{R}} S_{\boldsymbol{R}}^{\alpha} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \qquad , \qquad \hat{J}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} J(\boldsymbol{R}) e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \qquad , \qquad \hat{h}_{\boldsymbol{k}} = \frac{1}{N} \sum_{\boldsymbol{R}} h_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \qquad (1.94)$$

and their inverses

$$S_{\mathbf{R}}^{\alpha} = \frac{1}{N} \sum_{\mathbf{k}} S_{\mathbf{k}}^{\alpha} e^{i\mathbf{k}\cdot\mathbf{R}} \qquad , \qquad J(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} \hat{J}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}} \qquad h_{\mathbf{R}} = \sum_{\mathbf{k}} h_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} \qquad . \tag{1.95}$$

Note the placement of the 1/N factors differs in the definitions of $\hat{J}(\mathbf{k})$ and $\hat{h}_{\mathbf{k}}$. The commutation relations among the Fourier spin components are

$$[S_{k}^{+}, S_{k'}^{-}] = 2S_{k+k'}^{z} , \qquad [S_{k}^{z}, S_{k'}^{\pm}] = \pm S_{k+k'}^{\pm} .$$
(1.96)

We apply the Bogoliubov inequality of Eqn. 1.86 with

$$A = S_{-k_1}^- , \quad A^{\dagger} = S_{k_1}^+ , \quad C = S_{k_2}^+ , \quad C^{\dagger} = S_{-k_2}^- .$$
(1.97)

Thus, our version of the inequality may be written

$$\left| \left\langle \left[S_{-\boldsymbol{k}_{1}}^{-}, S_{\boldsymbol{k}_{2}}^{+} \right] \right\rangle \right|^{2} \leqslant \frac{1}{2} \beta \left\langle \left\{ S_{-\boldsymbol{k}_{1}}^{-}, S_{\boldsymbol{k}_{1}}^{+} \right\} \right\rangle \left\langle \left[S_{-\boldsymbol{k}_{2}}^{-}, \left[H, S_{\boldsymbol{k}_{2}}^{+} \right] \right] \right\rangle \quad , \tag{1.98}$$

Note that we may write $H = H_0 + H_1$ where

$$H_{0} = -\frac{1}{2N} \sum_{q} \hat{J}(q) \left\{ \frac{1}{2} S_{q}^{+} S_{-q}^{-} + \frac{1}{2} S_{q}^{-} S_{-q}^{+} + S_{q}^{z} S_{-q}^{z} \right\}$$

$$H_{1} = -\sum_{q} \hat{h}_{-q} S_{q}^{z} \quad .$$
(1.99)

We begin by computing the commutator

$$[H_0, S_{k_2}^+] = \frac{1}{2N} \sum_{q} \hat{J}(q) \left\{ S_q^+ S_{k_2-q}^z + S_{k_2+q}^z S_{-q}^+ - S_{k_2+q}^+ S_{-q}^z - S_q^z S_{k_2-q}^+ \right\} \quad , \tag{1.100}$$

from which we obtain, with a little work,

$$\left[S_{-\boldsymbol{k}_{2}}^{-}, \left[H_{0}, S_{\boldsymbol{k}_{2}}^{+}\right]\right] = \frac{1}{2N} \sum_{\boldsymbol{q}} \left(\hat{J}(\boldsymbol{q}) - \hat{J}(\boldsymbol{q} + \boldsymbol{k}_{2})\right) \left(S_{\boldsymbol{q}}^{+} S_{-\boldsymbol{q}}^{-} + S_{\boldsymbol{q}}^{-} S_{-\boldsymbol{q}}^{+} + 4S_{\boldsymbol{q}}^{z} S_{-\boldsymbol{q}}^{z}\right)$$
(1.101)

and where we have invoked $\sum_{k} \hat{J}(k) = 0$, which follows from the condition $J(\mathbf{0}) = 0$. Second we compute $[H_1, S_{k_2}^+] = -\sum_{q} \hat{h}_{-q} S_{q+k_2'}^+$ and thus

$$\left[S_{-k_2}^{-}, \left[H_1, S_{k_2}^{+}\right]\right] = 2\sum_{q} \hat{h}_{-q} S_{q}^{z} \quad .$$
(1.102)

Third, $[S_{-k_1}^-, S_{k_2}^+] = -S_{k_2-k_1}^z$. Finally, we have $\{S_{-k_1}^-, S_{k_1}^+\} = S_{-k_1}^- S_{k_1}^+ + S_{k_1}^+ S_{-k_1}^-$. Note that $\left|\left\langle [S_{-k_1}^-, S_{k_2}^+] \right\rangle\right|^2 = \left|\left\langle S_{k_2-k_1}^z \right\rangle\right|^2 = N^2 \left|\hat{m}_{k_2-k_1}\right|^2$. (1.103)

We define the quantity $\Gamma({m k}_2)\equiv\Gamma_0({m k}_2)+\Gamma_1({m k}_2)$, where

$$\Gamma_{0}(\mathbf{k}_{2}) = \left[S_{-\mathbf{k}_{2}}^{-}, [H_{0}, S_{\mathbf{k}_{2}}^{+}]\right] \\
= \frac{1}{2N} \sum_{\mathbf{q}} \left(\hat{J}(\mathbf{q}) - \frac{1}{2}\hat{J}(\mathbf{q} + \mathbf{k}_{2}) - \frac{1}{2}\hat{J}(\mathbf{q} - \mathbf{k}_{2})\right) \left\langle 4S_{\mathbf{q}}^{z}S_{-\mathbf{q}}^{z} + S_{\mathbf{q}}^{+}S_{-\mathbf{q}}^{-} + S_{\mathbf{q}}^{-}S_{-\mathbf{q}}^{+}\right\rangle \\
= \sum_{\mathbf{R}_{1}, \mathbf{R}_{2}} J(\mathbf{R}_{1}) \left(1 - \cos(\mathbf{k}_{2} \cdot \mathbf{R}_{1})\right) \left\langle S_{\mathbf{R}_{2}}^{x}S_{\mathbf{R}_{1} + \mathbf{R}_{2}}^{x} + S_{\mathbf{R}_{2}}^{y}S_{\mathbf{R}_{1} + \mathbf{R}_{2}}^{y} + 2S_{\mathbf{R}_{2}}^{z}S_{\mathbf{R}_{1} + \mathbf{R}_{2}}^{z}\right) \tag{1.104}$$

and

$$\Gamma_1(\mathbf{k}_2) = \left\langle \left[S^-_{-\mathbf{k}_2}, \left[H_0, S^+_{\mathbf{k}_2} \right] \right] \right\rangle = 2N \sum_{\mathbf{q}} \hat{h}_{-\mathbf{q}} \, \hat{m}_{\mathbf{q}} \quad .$$
(1.105)

We may now easily derive the following bounds:

$$\Gamma_{0}(\mathbf{k}_{2}) \leqslant NS(S + \frac{1}{2}) \, \mathbf{k}_{2}^{2} \sum_{\mathbf{R}} \mathbf{R}^{2} J(\mathbf{R}) \equiv 4N \mathcal{J} \, \mathbf{k}_{2}^{2} \, a^{2}
\Gamma_{1}(\mathbf{k}_{2}) \leqslant 2N \sum_{\mathbf{q}} |\hat{h}_{-\mathbf{q}}| \cdot |\hat{m}_{\mathbf{q}}| \quad .$$
(1.106)

with $\mathcal{J} \equiv \frac{1}{4}S(S+\frac{1}{2})\sum_{\mathbf{R}}(\mathbf{R}/a)^2 J(\mathbf{R})$, where we presume a *d*-dimensional cubic lattice of lattice constant *a*.

We are almost ready to claim our prize. At this point we have the inequality

$$\left\langle S_{\boldsymbol{K}-\boldsymbol{k}_{2}}^{-}S_{\boldsymbol{k}_{2}-\boldsymbol{K}}^{+}+S_{\boldsymbol{k}_{2}-\boldsymbol{K}}^{+}S_{\boldsymbol{K}-\boldsymbol{k}_{2}}^{-}\right\rangle \geqslant \frac{N}{2\beta} \cdot \frac{|\hat{m}_{\boldsymbol{K}}|^{2}}{\mathcal{J}\boldsymbol{k}_{2}^{2}\,a^{2}+\frac{1}{2}\sum_{\boldsymbol{q}}|\hat{h}_{-\boldsymbol{q}}|\cdot|\hat{m}_{\boldsymbol{q}}|} \quad , \tag{1.107}$$

with $\mathbf{k}_1 \equiv \mathbf{k}_2 - \mathbf{K}$. We now sum both sides of the equation over \mathbf{k}_2 , which owing to presumed periodic boundary conditions takes a discrete set of values $\mathbf{k}_2 = (2\pi n_1/N_1 a, 2\pi n_2/N_2 a, 2\pi n_3/N_3 a)$, with $N = N_1 N_2 N_3$ where $n_j \in \{1, \ldots, N_j\}$. The system is thus a cubic rectangle of dimensions $N_1 \times N_2 \times N_3$ cells, with each cell of volume a^3 . On the LHS, we obtain

$$\sum_{k_2} \left\langle S_{K-k_2}^- S_{k_2-K}^+ + S_{k_2-K}^+ S_{K-k_2}^- \right\rangle = 2N \sum_{R} \left\langle (S_R^x)^2 + (S_R^y)^2 \right\rangle < 2N^2 S(S+1) \quad .$$
(1.108)

Thus,

$$|\hat{m}_{K}|^{2} < \frac{4S(S+1)}{k_{\rm B}T} \bigg/ a^{d}_{\hat{\Omega}} \int \frac{d^{d}k}{(2\pi)^{d}} \frac{1}{\mathcal{J}k^{2}a^{2} + \frac{1}{2}\sum_{q}|\hat{h}_{-q}| \cdot |\hat{m}_{q}|}$$
(1.109)

Consider the case where $\hat{h}_q = \hat{h}_{-K} \delta_{q,-K} + \hat{h}_K \delta_{q,K}$. The Brillouin zone is a *d*-dimensional cube of side length $2\pi/a$. We are free to *underestimate* the integral, since this *overestimates* the RHS of the above inequality, and to this end we integrate instead over a *d*-dimensional sphere of radius $b = \pi/a$, yielding

$$|\hat{m}_{K}|^{2} < \frac{4S(S+1)}{k_{\rm B}T} \bigg/ \frac{\Omega_{d}}{(2\pi)^{d}} \int_{0}^{\pi} \frac{du \, u^{d-1}}{\mathcal{J}u^{2} + |\hat{h}_{K}| \cdot |\hat{m}_{K}|} \quad , \tag{1.110}$$

where $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the total solid angle in d space dimensions and $u = |\mathbf{k}|a$. We simplify notion by defining $h \equiv |\hat{h}_K|$ and $m \equiv |\hat{m}_K|$. We may now derive the following inequalities.

$$d = 1 : \quad m < C_1 \left(\frac{h\mathcal{J}}{(k_{\rm B}T)^2}\right)^{1/3}$$

$$d = 2 : \quad m < C_2 \frac{(\mathcal{J}/k_{\rm B}T)^{1/2}}{\ln^{1/2}(\mathcal{J}/hm)}$$

$$h = 0, \ d > 2 : \quad m < C_d \ \mathcal{J}/k_{\rm B}T \quad ,$$

(1.111)

where the $C_{1,2,\dots}$ are numerical constants. In the limit $h \to 0$, we see that m must vanish for d = 1 and d = 2. For d > 2, there is no such requirement.

1.5.4 Goldstone's theorem

Goldstone's theorem says that whenever the ground state $|\Psi_0\rangle$ of a thermodynamically large quantum system (or QFT) breaks a continuous symmetry of the Hamiltonian *H*, there is a branch of gapless excitations in the spectrum of *H*, known as *Goldstone bosons*. Let's illustrate this phenomenon with the explicit example of the spin-*S* quantum Heisenberg ferromagnet,

$$H = -\sum_{i < j} J_{ij} \, \boldsymbol{S}_i \cdot \boldsymbol{S}_i \quad . \tag{1.112}$$

We assume $J_{ij} = J(\mathbf{R}_i - \mathbf{R}_j) > 0$, *i.e.* the system is ferromagnetic, preferring all pairs of interacting spins to align. Each component of the total spin operator $\mathbf{S} = \sum_i S_i$ commutes with each term of *H*, *i.e.*

$$\left[\mathcal{S}^{\alpha}, \mathbf{S}_{i} \cdot \mathbf{S}_{j}\right] = 0 \tag{1.113}$$

because $S_i \cdot S_j$ is rotationally invariant and the S^{α} are the generators of rotations. The global symmetry group is SU(2), which is continuous. It is clear that any state $|\Psi_0\rangle$ for which $S_i \cdot S_j |\Psi_0\rangle = S^2 |\Psi_0\rangle$ is a ground state of H, since each individual term in the sum is separately minimized. The ground state energy is then $E_0 = -\frac{1}{2}N\hat{J}(\mathbf{0})S^2$, where $\hat{J}(\mathbf{k}) = \sum_{\mathbf{R}} J(\mathbf{R}) e^{-i\mathbf{k}\cdot\mathbf{R}}$.

Consider then the state $|\Uparrow\rangle$ in which $S_i^z |\Uparrow\rangle = S |\Uparrow\rangle$, *i.e.* all spins maximally polarized in the \hat{z} direction. Clearly $|\Uparrow\rangle$ is a ground state. But so is $|\Downarrow\rangle$. Indeed, so is any state of the form $|\Psi_0(\hat{n})\rangle = \bigotimes_i |\hat{n}\rangle_i$ in which each spin is in a coherent state maximally polarized along the direction \hat{n} , *i.e.* $\hat{n} \cdot S_i |\Psi_0(\hat{n})\rangle = S |\Psi_0(\hat{n})\rangle^{25}$. Thus, we have an entire manifold of states, all with energy E_0 , corresponding to total spin S = NS. The degeneracy of this ground state sector is S(S + 1), and states with different values of S^z are of course orthogonal. In the coherent state basis, we have

$$\left| \left\langle \Psi_0(\hat{\boldsymbol{n}}) \left| \Psi_0(\hat{\boldsymbol{n}}') \right\rangle \right|^2 = \left(\frac{1 + \hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{n}}'}{2} \right)^N \quad , \tag{1.114}$$

where *N* is the total number of spins. In the thermodynamic limit, these states are *macroscopi*cally distinct

$$\left|\left\langle \Psi_{0}(\hat{\boldsymbol{n}}) \left| \mathcal{O}_{i} \mathcal{O}_{j} \right| \Psi_{0}(\hat{\boldsymbol{n}}') \right\rangle\right|^{2} = \left(\frac{1 + \hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{n}}'}{2}\right)^{N-2} \left|\left\langle \hat{\boldsymbol{n}}, \hat{\boldsymbol{n}} \right| \mathcal{O}_{i} \mathcal{O}_{j} \left| \hat{\boldsymbol{n}}, \hat{\boldsymbol{n}} \right\rangle\right|^{2} , \qquad (1.115)$$

which vanishes in the thermodynamic limit.

Next, consider the operator $S^{\alpha}(\mathbf{k}) = N^{-1} \sum_{i} S_{i}^{\alpha} e^{-i\mathbf{k}\cdot\mathbf{R}_{i}}$, which we met in Eqn. 1.95. It is straightforward to derive the result

$$[H, \mathcal{S}^{-}(\mathbf{k})] = \sum_{i,j} J(\mathbf{R}_i - \mathbf{R}_j) \left(1 - e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)}\right) S_j^{-} e^{-i\mathbf{k}\cdot\mathbf{R}_j} S_i^z \quad .$$
(1.116)

²⁵In this notation, our previously defined state $|\Psi_0\rangle = |\uparrow\rangle$ is expressed as $|\Psi_0\rangle = |\Psi_0(\hat{z})\rangle$.

We assume that the diagonal elements of J_{ij} all vanish, *i.e.* $J(\mathbf{0}) = \sum_{k} \hat{J}(k) = 0$. The above identity, acting on the state $|\uparrow\rangle$, then yields

$$[H, \mathcal{S}^{-}(\mathbf{k})] | \Uparrow \rangle = S \left[\hat{J}(\mathbf{0}) - \hat{J}(\mathbf{k}) \right] \mathcal{S}^{-}(\mathbf{k}) | \Uparrow \rangle \quad , \tag{1.117}$$

which establishes that $S_k^- | \uparrow \rangle$ is an *eigenstate* of H, with eigenvalue $E_k = E_0 + S[\hat{J}(\mathbf{0}) - \hat{J}(\mathbf{k})]$. Thus, the excitation spectrum of this branch, which has one state for each wavevector \mathbf{k} , is

$$\hbar\omega_{k} = E_{k} - E_{0} = S[\hat{J}(\mathbf{0}) - \hat{J}(\mathbf{k})]$$
 (1.118)

These excitations are called *spin waves*, and they are examples of Goldstone bosons. Note that the k = 0 spin wave state,

$$\mathcal{S}^{-}(\mathbf{0})\left|\Uparrow\right\rangle = \sum_{i} S_{i}^{-}\left|\Uparrow\right\rangle \quad , \tag{1.119}$$

is among the ground state manifold, with total spin S = NS and polarization $S^{z} = NS - 1$.

Note that in systems with a discrete symmetry, such as the Ising model, with symmetry group \mathbb{Z}_2 , there are in general no Goldstone bosons. For the Ising ferromagnet $H = -\sum_{i < j} J_{ij} \sigma_i \sigma_j$, where each $\sigma_i = \pm 1$, there are two degenerate ground states, $|\uparrow\rangle$ and $|\downarrow\rangle$, each of which has total energy $E_0 = -\frac{1}{2}N\hat{J}(\mathbf{0})$. In dimensions d > 1, the lowest-lying excitation in either case is a single spin flip, with excitation energy $\Delta E = 2\hat{J}(\mathbf{0})$. (In d = 1, with nearest-neighbor interactions, the lowest-lying excitation is a domain wall, with energy $\hat{J}(\mathbf{0}) = 2J$.)

Field theories and Goldstone's theorem

Consider the $|\phi|^4$ field theory for the real *n*-component field $\phi = (\phi^1, \dots, \phi^n)$, with relativistic Lagrangian density

$$\mathcal{L} = \frac{1}{2} (\partial_{\mu} \phi) (\partial^{\mu} \phi) - \frac{1}{2} m^2 \phi^2 - \frac{1}{4} \lambda (\phi^2)^2 \quad .$$
 (1.120)

The metric used to raise and lower indices is $g_{\mu\nu} = \text{diag}(+, -, \dots, -)$. The equations of motion are found to be

$$\partial_{\mu}\partial^{\mu}\phi + m^{2}\phi + \lambda \phi^{2}\phi = 0 \quad . \tag{1.121}$$

If $m^2 > 0$, we can obtain solutions when $|\phi| \ll 1$ by dropping the cubic term. The solutions are plane waves: $\phi(x, t) = A e^{i(k \cdot x - \omega t)}$ where $\omega^2 = k^2 + m^2$. The spectrum is massive.

What happens when $m^2 < 0$? In this case the potential $V(\phi) = \frac{1}{2}m^2\phi^2 + \frac{1}{4}\lambda(\phi^2)^2$ is minimized when $|\phi| = \phi_0 = \sqrt{-m^2/\lambda}$. Let's write $\phi = \phi_0 (1 + \eta)^{1/2} \hat{\omega}$, where $\hat{\omega}$ is a unit vector. One then obtains

$$\mathcal{L} = \frac{1}{8}\phi_0^2 \frac{(\partial_\mu \eta)(\partial^\mu \eta)}{1+\eta} + \frac{1}{2}\phi_0^2 (1+\eta)(\partial_\mu \hat{\omega})(\partial^\mu \hat{\omega}) - \frac{1}{4}m^2\phi_0^2 (1-\eta^2) \quad .$$
(1.122)

The linearized EL equations are then

$$\partial_{\mu}\partial^{\mu}\eta = 2m^{2}\eta$$

$$\partial_{\mu}\partial^{\mu}\hat{\omega} = 0 \quad . \tag{1.123}$$

1.5. FOUR VIGNETTES

The first equation results in a massive relativistic dispersion $\omega^2 = \mathbf{k}^2 + 2m^2$, while the second, as we have seen, yields gapless solutions with $\omega = |\mathbf{k}|$, which are the Goldstone bosons. Note that if ϕ has n = 1 component, then there is no $\hat{\boldsymbol{\omega}}$ field and there are no Goldstone bosons.

Consider next the example of the nonrelativistic complex $|\psi|^4$ theory, otherwise known as the Gross-Pitaevskii model, with

$$\mathcal{L} = i\hbar \,\bar{\psi} \,\partial_t \,\psi - \frac{\hbar^2}{2m} \,|\boldsymbol{\nabla}\psi|^2 - \frac{1}{2}g \left(|\psi|^2 - n_0\right)^2 \tag{1.124}$$

We write $\psi = \sqrt{n_0} \left(1 + \eta \right) e^{i\xi}$, which yields

$$\mathcal{L} = -\hbar n_0 (1+\eta)^2 \partial_t \xi - \frac{\hbar^2 n_0}{2m} (\nabla \eta)^2 - \frac{\hbar^2 n_0}{2m} (1+\eta)^2 (\nabla \xi)^2 - \frac{1}{2} g n_0^2 (4\eta^2 + 4\eta^3 + \eta^4) \quad . \quad (1.125)$$

The linearized equations of motion are then found to be

$$-2\hbar n_0 \partial_t \xi = -\frac{\hbar^2 n_0}{m} \nabla^2 \eta + 4g n_0^2 \eta$$

+
$$2\hbar n_0 \partial_t \eta = -\frac{\hbar^2 n_0}{m} \nabla^2 \xi \quad .$$
(1.126)

We now obtain plane wave solutions of the form

$$\begin{pmatrix} \eta(\boldsymbol{x},t)\\ \xi(\boldsymbol{x},t) \end{pmatrix} = \begin{pmatrix} \hat{\eta}\\ \hat{\xi} \end{pmatrix} e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} \quad , \tag{1.127}$$

which, when inserted into the EL equations, yields the pair

$$2i\hbar\omega\,\hat{\xi} = \left(\frac{\hbar^2 \mathbf{k}^2}{m} + 4gn_0\right)\hat{\eta}$$

$$-2i\hbar\omega\,\hat{\eta} = \frac{\hbar^2 \mathbf{k}^2}{m}\hat{\xi} \quad .$$
(1.128)

The solutions are

$$\omega = \pm c \, |\mathbf{k}| \sqrt{1 + \frac{\hbar^2 \mathbf{k}^2}{4m^2 c^2}} \quad . \tag{1.129}$$

Note that as $\mathbf{k} \to 0$ we obtain a massless relativistic dispersion $\omega = \pm c |\mathbf{k}|$, while for $|\mathbf{k}| \to \infty$ we recover the ballistic dispersion $\omega = \hbar \mathbf{k}^2/2m$. These massless excitations are Goldstone modes of the broken U(1) symmetry and correspond to phonons in a superfluid.

Finally, let's get crazy and consider the *gauged*, relativistic $|\psi|^4$ theory, with

$$\mathcal{L} = \frac{1}{2g} \left(\partial_{\mu} + ieA_{\mu} \right) \bar{\psi} \left(\partial^{\mu} + ieA^{\mu} \right) \psi - \frac{m^2}{2gn_0} \left(\bar{\psi}\psi - n_0 \right)^2 - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \quad , \tag{1.130}$$



Figure 1.15: Left: double well potential $V(\phi)$ for the scalar field $\phi \in \mathbb{R}$. Right: Mexican hat potential for the complex scalar field $\phi \in \mathbb{C}$ with $V(\phi, \bar{\phi}) = \frac{1}{2}m^2(|\phi|^2 - n_0)^2$.

where the field strength tensor is written in terms of the gauge field as $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$. This theory has a *local gauge symmetry* whereby the combined operations

$$\psi \to \psi e^{i\alpha} \quad , \qquad A_{\mu} \to A_{\mu} - e^{-1} \partial_{\mu} \alpha \quad ,$$
 (1.131)

where $\alpha(\boldsymbol{x}, t)$ is a field, leaves \mathcal{L} invariant.

If we drop the gauge field, *i.e.* set e = 0, we may again expand about one of the local minima at $|\psi| = n_0^{1/2}$, writing

$$\psi = \sqrt{n_0} (1+\eta) e^{i\xi} \quad , \tag{1.132}$$

as above. Then

$$\mathcal{L} = \frac{n_0}{2g} (\partial_\mu \eta) (\partial^\mu \eta) + \frac{n_0}{2g} (1+\eta)^2 (\partial_\mu \xi) (\partial^\mu \xi) - \frac{m^2 n_0}{2g} (4\eta^2 + 4\eta^3 + \eta^4) \quad .$$
(1.133)

The linearized equations of motion are then

$$\partial_{\mu}\partial^{\mu}\eta = (2m)^{2}\eta \qquad , \qquad \partial_{\mu}\partial^{\mu}\xi = 0 \quad ,$$
 (1.134)

yielding two modes. The η mode carries a massive relativistic dispersion $\omega^2 = \mathbf{k}^2 + (2m)^2$, while the ξ mode is the gapless Goldstone boson with $\omega^2 = \mathbf{k}^2$.

When $e \neq 0$, we may take advantage of the gauge invariance to define a shifted gauge field

$$\widetilde{A}_{\mu} \equiv A_{\mu} - e^{-1} \partial_{\mu} \xi \quad . \tag{1.135}$$

The transformed Lagrangian becomes

$$\mathcal{L} = \frac{n_0}{2g} \left(\partial_\mu \eta \right) \left(\partial^\mu \eta \right) + \frac{n_0 e^2}{2g} \left(1 + \eta \right)^2 \widetilde{A}_\mu \widetilde{A}^\mu - \frac{m^2 n_0}{2g} \left(4\eta^2 + 4\eta^3 + \eta^4 \right) - \frac{1}{4} \widetilde{F}_{\mu\nu} \widetilde{F}^{\mu\nu} \quad , \qquad (1.136)$$

from which we can read off the following features:

- The photon has become a massive triplet \widetilde{A}_{μ} , with $m_{\widetilde{A}} = e\sqrt{n_0/g}$.
- There is no ξ particle! It has been *eaten* by the photon field.
- The Higgs field η has a mass which is independent of e, with $m_n = 2m$.

To reiterate what we have learned in this section: Classically, a particle in a double well potential exhibits spontaneous symmetry breaking. It *must* choose which well in which to lie. But quantum mechanically, we know that the ground state is a symmetric superposition of left and right well states. A similar consideration holds in the case of continuous symmetries, for the Mexican hat potential. A classical particle will minimize its energy at any point along the trough of the potential, but the quantum ground state is a rotationally symmetric *s*-wave state with no nodes. In a field theory setting, there are an *infinite number* of degrees of freedom, and the double well or Mexican hat exists *at every point in space*. This kills tunneling between the different broken symmetry 'pure' states, *viz*. $\langle L | R \rangle \sim \langle \varphi_L | \varphi_R \rangle^V \to 0$ in the $V \to \infty$ limit of infinite system volume. This state of affairs is described in Fig. 1.15.

1.6 Appendix : The Foldy-Wouthuysen Transformation

1.6.1 The Dirac Hamiltonian

Let us write

$$\hat{H} = mc^2 \gamma^0 + c\gamma^0 \gamma \cdot \pi + V , \qquad (1.137)$$

where

$$\pi = p + \frac{e}{c}A \tag{1.138}$$

is the dynamical momentum and where the γ^{μ} are the Dirac matrices,

$$\gamma^{0} = \begin{pmatrix} 1_{2\times 2} & 0_{2\times 2} \\ 0_{2\times 2} & -1_{2\times 2} \end{pmatrix} , \qquad \gamma = \begin{pmatrix} 0_{2\times 2} & \boldsymbol{\sigma}_{2\times 2} \\ -\boldsymbol{\sigma}_{2\times 2} & 0_{2\times 2} \end{pmatrix} .$$
(1.139)

Here σ is the vector of Pauli matrices.

The idea behind the FW transformation is to unitarily transform to a different Hilbert space basis such that the coupling in \hat{H} between the upper and lower components of the Dirac spinor vanishes. This may be done systematically as an expansion in inverse powers of the electron mass m. We begin by defining $K \equiv c\gamma^0 \gamma \cdot \pi + V$ so that $\hat{H} = mc^2 \gamma^0 + K$. Note that K is of order m^0 . We then write

$$\hat{\hat{H}} = e^{iS} \hat{H} e^{-iS} = \hat{H} + i [S, \hat{H}] + \frac{(i)^2}{2!} [S, [S, \hat{H}]] + \dots ,$$
(1.140)

where S itself is written as a power series in $(mc^2)^{-1}$:

$$S = \frac{S_0}{mc^2} + \frac{S_1}{(mc^2)^2} + \dots$$
 (1.141)

The job now is to write \hat{H} as a power series in m^{-1} . The first few terms are easy to find:

$$\tilde{\hat{H}} = mc^2 \gamma^0 + K + i [S_0, \gamma^0] + \frac{1}{mc^2} \left(i [S_0, K] + i [S_1, \gamma^0] - \frac{1}{2} [S_0, [S_0, \gamma^0]] \right) + \dots$$
(1.142)

We choose the operators S_n so as to cancel, at each order in m^{-1} , the off-diagonal terms in \hat{H} that couple the upper two components of Ψ to the lower two components of Ψ . To order m^0 , we then demand

$$c\gamma^0 \boldsymbol{\gamma} \cdot \boldsymbol{\pi} + i [S_0, \gamma^0] = 0.$$
(1.143)

Note that we do not demand that $i[S_0, \gamma^0]$ completely cancel K – indeed it is impossible to find such an S_0 , and one way to see this is to take the trace. The trace of any commutator must vanish, but Tr K = 4V, which is in general nonzero. But this is of no concern to us, since we only need cancel the (traceless) *off-diagonal* part of K, which is to say $c\gamma^0\gamma \cdot \pi$.

To solve for S_0 , one can write it in terms of its four 2×2 subblocks, compute the commutator with γ^0 , and then impose eqn. 1.143. One then finds $S_0 = -\frac{i}{2}c \gamma \cdot \pi$.

STUDENT EXERCISE: Derive the result $S_0 = -\frac{i}{2}c \gamma \cdot \pi$.

At the next level, we have to deal with the term in the round brackets in eqn. 1.142. Since we know S_0 , we can compute the first and the third terms therein. In general, this will leave us with an off-diagonal term coupling upper and lower components of Ψ . We then choose S_1 so as to cancel this term. This calculation already is tedious, and we haven't even gotten to the spin-orbit interaction term yet, since it is of order m^{-2} .

1.6.2 Emergence of the spin-orbit and Zeeman interaction terms

Here's a simpler way to proceed to order m^{-2} . Let a, b be block indices and i, j be indices within each block. Thus, the component Ψ_{ai} is the i^{th} component of the a^{th} block; $\Psi_{a=1,i=2}$ is the lower component of the upper block, *i.e.* the second component of the four-vector Ψ .

Write the Hamiltonian as

$$\hat{H} = mc^2 \tau^z + c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \tau^x + V(\boldsymbol{r}) , \qquad (1.144)$$

where τ^{μ} are Pauli matrices with indices a, b and σ^{ν} are Pauli matrices with indices i, j. The σ and τ matrices commute because they act on different indices.

A very important result regarding Pauli matrices:

$$e^{i\theta\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\tau}/2}\,\tau^{\alpha}\,e^{-i\theta\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\tau}/2} = n^{\alpha}n^{\beta}\,\tau^{\beta} + \cos\theta\,(\delta^{\alpha\beta} - n^{\alpha}n^{\beta})\,\tau^{\beta} + \sin\theta\,\epsilon^{\alpha\beta\gamma}\,n^{\beta}\,\tau^{\gamma}\,.$$
(1.145)

STUDENT EXERCISE: Verify and interpret the above result.

Using this result, we can write

$$A \tau^{z} + B \tau^{x} = \sqrt{A^{2} + B^{2}} \cdot e^{-i \tan^{-1}(B/A) \tau^{y}/2} \tau^{z} e^{i \tan^{-1}(B/A) \tau^{y}/2} , \qquad (1.146)$$

and, for our specific purposes,

$$mc^{2}\tau^{z} + c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \tau^{x} = \sqrt{(mc^{2})^{2} + (c\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^{2}} \cdot U \tau^{z} U^{\dagger} , \qquad (1.147)$$

where

$$U = \exp\left\{-\frac{i}{2}\tan^{-1}\left(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{mc}\right)\tau^{y}\right\}.$$
(1.148)

The fact that $\boldsymbol{\sigma} \cdot \boldsymbol{\pi}$ is an operator is no obstacle here, since it commutes with the τ^{μ} matrices. We can give meaning to expressions like $\tan^{-1}(\boldsymbol{\sigma} \cdot \boldsymbol{\pi}/mc)$ in terms of their Taylor series expansions.

We therefore have the result,

$$U^{\dagger} \hat{H} U = \sqrt{(mc^2)^2 + (c\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2} \cdot \tau^z + U^{\dagger} V(\boldsymbol{r}) U .$$
 (1.149)

The first term is diagonal in the block indices. Expanding the square root, we have

$$mc^{2}\sqrt{1 + \left(\frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{mc}\right)^{2}} = mc^{2} + \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^{2}}{2m} + \mathcal{O}(m^{-3})$$

$$= mc^{2} + \frac{\boldsymbol{\pi}^{2}}{2m} + \frac{e\hbar}{2mc} \boldsymbol{B} \cdot \boldsymbol{\sigma} + \mathcal{O}(m^{-3}), \qquad (1.150)$$

since

$$(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2 = \sigma^{\mu} \sigma^{\nu} \pi^{\mu} \pi^{\nu} = (\delta^{\mu\nu} + i\epsilon^{\mu\nu\lambda} \sigma^{\lambda}) \pi^{\mu} \pi^{\nu}$$

$$= \pi^2 + \frac{i}{2} \epsilon^{\mu\nu\lambda} \left[p^{\mu} + \frac{e}{c} A^{\mu}, p^{\nu} + \frac{e}{c} A^{\nu} \right] = \pi^2 + \frac{e\hbar}{c} \boldsymbol{B} \cdot \boldsymbol{\sigma} .$$
(1.151)

We next need to compute $U^{\dagger}V(\mathbf{r})U$ to order m^{-2} . To do this, first note that

$$U = 1 - \frac{i}{2} \frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{mc} \tau^{y} - \frac{1}{8} \left(\frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{mc}\right)^{2} + \dots , \qquad (1.152)$$

Thus,

$$U^{\dagger} V U = V + \frac{i}{2mc} \left[\boldsymbol{\sigma} \cdot \boldsymbol{\pi}, V \right] \tau^{y} - \frac{1}{8m^{2}c^{2}} \left[\boldsymbol{\sigma} \cdot \boldsymbol{\pi}, \left[\boldsymbol{\sigma} \cdot \boldsymbol{\pi}, V \right] \right] + \dots$$
(1.153)

Upon reflection, one realizes that, to this order, it suffices to take the first term in the Taylor expansion of $\tan^{-1}(\sigma \cdot \pi/mc)$ in eqn. 1.148, in which case one can then invoke eqn. 1.140 to

obtain the above result. The second term on the RHS of eqn. 1.153 is simply $\frac{\hbar}{2mc} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V \tau^y$. The third term is

$$\frac{i\hbar}{8m^2c^2} \left[\sigma^{\mu}\pi^{\mu}, \sigma^{\nu}\partial^{\nu}V \right] = \frac{i\hbar}{8m^2c^2} \left\{ \sigma^{\mu} \left[\pi^{\mu}, \sigma^{\nu}\partial^{\nu}V \right] + \left[\sigma^{\mu}, \sigma^{\nu}\partial^{\nu}V \right] \pi^{\mu} \right\} \\
= \frac{i\hbar}{8m^2c^2} \left\{ \frac{\hbar}{i}\partial^{\mu}\partial^{\nu}V \sigma^{\mu}\sigma^{\nu} + 2i\epsilon^{\mu\nu\lambda}\sigma^{\lambda}\partial^{\nu}V \pi^{\mu} \right\} \\
= \frac{\hbar^2}{8m^2c^2} \nabla^2 V + \frac{\hbar}{4m^2c^2} \sigma \cdot \nabla V \times \pi .$$
(1.154)

Therefore,

$$U^{\dagger} \hat{H} U = \left(mc^{2} + \frac{\pi^{2}}{2m} + \frac{e\hbar}{2mc} \mathbf{B} \cdot \boldsymbol{\sigma} \right) \tau^{z} + V + \frac{\hbar}{2mc} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V \tau^{y} + \frac{\hbar^{2}}{8m^{2}c^{2}} \boldsymbol{\nabla}^{2} V + \frac{\hbar}{4m^{2}c^{2}} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V \times \boldsymbol{\pi} + \mathcal{O}(m^{-3}) .$$

$$(1.155)$$

This is not block-diagonal, owing to the last term on the RHS of the top line. We can eliminate this term by effecting yet another unitary transformation. However, this will result in a contribution to the energy of order m^{-3} , so we can neglect it. To substantiate this last claim, drop all the block-diagonal terms except for the leading order one, $mc^2 \tau^z$, and consider the Hamiltonian

$$\mathcal{K} = mc^2 \,\tau^z + \frac{\hbar}{2mc} \,\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \, V \,\tau^y \,. \tag{1.156}$$

We now know how to bring this to block-diagonal form. The result is

$$\tilde{\mathcal{K}} = mc^2 \sqrt{1 + \left(\frac{\hbar \,\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V}{2m^2 c^3}\right)^2} \, \tau^z = \left(mc^2 + \frac{\hbar^2 (\boldsymbol{\nabla} V)^2}{8m^3 c^4} + \dots\right) \tau^z \,, \tag{1.157}$$

and the correction is of order m^{-3} , as promised.

We now assume all the negative energy $(\tau^z = -1)$ states are filled. The Hamiltonian for the electrons, valid to $\mathcal{O}(m^{-3})$, is then

$$\tilde{\hat{H}} = mc^2 + V + \frac{\pi^2}{2m} + \frac{e\hbar}{2mc} \mathbf{B} \cdot \boldsymbol{\sigma} + \frac{\hbar^2}{8m^2c^2} \nabla^2 V + \frac{\hbar}{4m^2c^2} \boldsymbol{\sigma} \cdot \nabla V \times \boldsymbol{\pi} .$$
(1.158)

1.7 Appendix : Ideal Bose Gas Condensation

We begin with the grand canonical Hamiltonian $K = H - \mu N$ for the ideal Bose gas,

$$K = \sum_{k} (\varepsilon_{k} - \mu) b_{k}^{\dagger} b_{k} - \sqrt{N} \sum_{k} \left(\nu_{k} b_{k}^{\dagger} + \bar{\nu}_{k} b_{k} \right) \quad .$$
(1.159)

Here b_k^{\dagger} is the creation operator for a boson in a state of wavevector k, hence $[b_k, b_{k'}^{\dagger}] = \delta_{kk'}$. The dispersion relation is given by the function ε_k , which is the energy of a particle with wavevector k. We must have $\varepsilon_k - \mu \ge 0$ for all k, lest the spectrum of K be unbounded from below. The fields $\{\nu_k, \bar{\nu}_k\}$ break a global O(2) symmetry.

Students who have not taken a course in solid state physics can skip the following paragraph, and be aware that $N = V/v_0$ is the total volume of the system in units of a fundamental "unit cell" volume v_0 . The thermodynamic limit is then $N \to \infty$. Note that N is not the boson particle number, which we'll call N_b .

Solid state physics boilerplate : We presume a setting in which the real space Hamiltonian is defined by some boson hopping on a Bravais lattice. The wavevectors \mathbf{k} are then restricted to the first Brillouin zone, $\hat{\Omega}$, and assuming periodic boundary conditions are quantized according to the condition $\exp(iN_l \mathbf{k} \cdot \mathbf{a}_l) = 1$ for all $l \in \{1, \ldots, d\}$, where \mathbf{a}_l is the l^{th} fundamental direct lattice vector and N_l is the size of the system in the \mathbf{a}_l direction; d is the dimension of space. The total number of unit cells is $N \equiv \prod_l N_l$. Thus, quantization entails $\mathbf{k} = \sum_l (2\pi n_l/N_l) \mathbf{b}_l$, where \mathbf{b}_l is the l^{th} elementary reciprocal lattice vector ($\mathbf{a}_l \cdot \mathbf{b}_{l'} = 2\pi \delta_{ll'}$) and n_l ranges over N_l distinct integers such that the allowed \mathbf{k} points form a discrete approximation to $\hat{\Omega}$.

To solve, we first shift the boson creation and annihilation operators, writing

$$K = \sum_{k} (\varepsilon_{k} - \mu) \,\beta_{k}^{\dagger} \beta_{k} - N \sum_{k} \frac{|\nu_{k}|^{2}}{\varepsilon_{k} - \mu} \quad , \qquad (1.160)$$

where

$$\beta_{k} = b_{k} - \frac{\sqrt{N}\nu_{k}}{\varepsilon_{k} - \mu} \qquad , \qquad \beta_{k}^{\dagger} = b_{k}^{\dagger} - \frac{\sqrt{N}\bar{\nu}_{k}}{\varepsilon_{k} - \mu} \qquad .$$
(1.161)

Note that $[\beta_k, \beta_{k'}^{\dagger}] = \delta_{kk'}$ so the above transformation is canonical. The Landau free energy $\Omega = -k_{\rm B}T \ln \Xi$, where $\Xi = \text{Tr } e^{-K/k_{\rm B}T}$, is given by

$$\Omega = Nk_{\rm B}T \int_{-\infty}^{\infty} d\varepsilon \ g(\varepsilon) \ln\left(1 - e^{(\mu - \varepsilon)/k_{\rm b}T}\right) - N \sum_{k} \frac{|\nu_{k}|^{2}}{\varepsilon_{k} - \mu} \quad , \tag{1.162}$$

where $g(\varepsilon)$ is the density of energy states per unit cell,

$$g(\varepsilon) = \frac{1}{N} \sum_{k} \delta(\varepsilon - \varepsilon_{k}) \xrightarrow[N \to \infty]{} v_{0} \int_{\hat{\Omega}} \frac{d^{d}k}{(2\pi)^{d}} \delta(\varepsilon - \varepsilon_{k}) \quad .$$
(1.163)

Note that

$$\psi_{k} \equiv \frac{1}{\sqrt{N}} \left\langle b_{k} \right\rangle = -\frac{1}{N} \frac{\partial \Omega}{\partial \bar{\nu}_{k}} = \frac{\nu_{k}}{\varepsilon_{k} - \mu} \quad . \tag{1.164}$$

In the condensed phase, ψ_k is nonzero.

The Landau free energy (grand potential) is a function $\Omega(T, N, \mu, \nu, \bar{\nu})$. We now make a Legendre transformation,

$$Y(T, N, \mu, \psi, \bar{\psi}) = \Omega(T, N, \mu, \nu, \bar{\nu}) + N \sum_{\boldsymbol{k}} \left(\nu_{\boldsymbol{k}} \bar{\psi}_{\boldsymbol{k}} + \bar{\nu}_{\boldsymbol{k}} \psi_{\boldsymbol{k}} \right) \quad . \tag{1.165}$$

Note that

$$\frac{\partial Y}{\partial \bar{\nu}_{k}} = \frac{\partial \Omega}{\partial \bar{\nu}_{k}} + N\psi_{k} = 0 \quad , \qquad (1.166)$$

by the definition of ψ_k . Similarly, $\partial Y / \partial \nu_k = 0$. We now have

$$Y(T, N, \mu, \psi, \bar{\psi}) = Nk_{\rm B}T \int_{-\infty}^{\infty} d\varepsilon \ g(\varepsilon) \ln\left(1 - e^{(\mu - \varepsilon)/k_{\rm b}T}\right) + N\sum_{k} (\varepsilon_{k} - \mu) |\psi_{k}|^{2} \quad .$$
(1.167)

Therefore, the boson particle number per unit cell is given by the *dimensionless density*,

$$n = \frac{N_b}{N} = -\frac{1}{N} \frac{\partial Y}{\partial \mu} = \sum_{k} |\psi_k|^2 + \int_{-\infty}^{\infty} d\varepsilon \, \frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_{\rm B}T} - 1} \quad , \tag{1.168}$$

and the relation between the condensate amplitude ψ_k and the field ν_k is given by

$$\nu_{k} = \frac{1}{N} \frac{\partial Y}{\partial \bar{\psi}_{k}} = (\varepsilon_{k} - \mu) \psi_{k} \quad . \tag{1.169}$$

Recall that ν_k acts as an external field. Let the dispersion ε_k be minimized at k = K. Without loss of generality, we may assume this minimum value is $\varepsilon_K = 0$. We see that if $\nu_k = 0$ then one of two must be true:

- (i) $\psi_{k} = 0$ for all k
- (ii) $\mu = \varepsilon_{K}$, in which case ψ_{K} can be nonzero.

Thus, for $\nu = \bar{\nu} = 0$ and $\mu > 0$, we have the usual equation of state,

$$n(T,\mu) = \int_{-\infty}^{\infty} d\varepsilon \, \frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_{\rm B}T} - 1} \quad , \tag{1.170}$$

which relates the intensive variables *n*, *T*, and μ . When $\mu = 0$, the equation of state becomes

$$n(T, \mu = 0) = \overbrace{K}^{n_0} |\psi_K|^2 + \overbrace{\int_{-\infty}^{\infty} d\varepsilon}^{n_>(T)} \frac{g(\varepsilon)}{e^{\varepsilon/k_{\rm B}T} - 1} \quad , \tag{1.171}$$

where now the sum is over only those K for which $\varepsilon_K = 0$. Typically this set has only one member, K = 0, but it is quite possible, due to symmetry reasons, that there are more such K values. This last equation of state is one which relates the intensive variables n, T, and n_0 , where

$$n_0 = \sum_{K} |\psi_K|^2$$
(1.172)

is the dimensionless condensate density. If the integral $n_>(T)$ in Eqn. 1.171 is finite, then for $n > n_0(T)$ we must have $n_0 > 0$. Note that, for any T, $n_>(T)$ diverges logarithmically whenever g(0) is finite. This means that Eqn. 1.170 can always be inverted to yield a finite $\mu(n, T)$, no matter how large the value of n, in which case there is no condensation and $n_0 = 0$. If $g(\varepsilon) \propto \varepsilon^{\alpha}$ with $\alpha > 0$, the integral converges and $n_>(T)$ is finite and monotonically increasing for all T. Thus, for fixed dimensionless number n, there will be a *critical temperature* T_c for which $n = n_>(T_c)$. For $T < T_c$, Eqn. 1.170 has no solution for any μ and we must appeal to eqn. 1.171. The condensate density, given by $n_0(n, T) = n - n_>(T)$, is then finite for $T < T_c$, and vanishes for $T \ge T_c$.

In the condensed phase, the phase of the order parameter ψ inherits its phase from the external field ν , which is taken to zero, in the same way the magnetization in the symmetry-broken phase of an Ising ferromagnet inherits its direction from an applied field *h* which is taken to zero. The important feature is that in both cases the applied field is taken to zero *after* the approach to the thermodynamic limit.

1.8 Appendix : Asymptotic Series in a Zero-Dimensional Field theory

In this appendix we will solve numerically for a zero-dimensional field theory, *i.e.* an integral $F(\lambda)$, which depends parametrically on a dimensionless parameter λ , with F(0) = 1, and compare the results with expansions from diagrammatic perturbation theory, We will see that the perturbation expansion is *asymptotic*, meaning that it is formally divergent, *i.e.* with a vanishing radius of convergence. However, if the results of summing the first N terms results in a relative error $S_N(\lambda) = R_N(\lambda)/F(\lambda)$, where $R_N(\lambda)$ is the remainder after N terms, is minimized by setting $N = N^*(\lambda)$, where $N^*(\lambda) \to \infty$ as $\lambda \to 0$.

Problem : The normalized Gaussian distribution $P(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ has the n^{th} moment

$$\langle x^n \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \ x^n \ e^{-x^2/2}$$

Clearly $\langle x^n \rangle = 0$ if *n* is a nonnegative odd integer. Next consider the *generating function*

$$Z(j) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \ e^{-x^2/2} \ e^{jx} = \exp\left(\frac{1}{2}j^2\right)$$

- (a) Show that $\langle x^n \rangle = (d^n Z/dj^n) |_{j=0}$ and provide an explicit result for $\langle x^{2k} \rangle$ where $k \in \mathbb{N}$.
- (b) Now consider the following integral:

$$F(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{1}{2} \, x^2 - \frac{\lambda}{4!} \, x^4\right) \,.$$

Clearly F(0) = 1, but for general $\lambda > 0$ the integral has no known analytic form²⁶, but we may express the result as a power series in the parameter λ by Taylor expanding $\exp(-\frac{\lambda}{4!}x^4)$ and then using the result of part (a) for the moments $\langle x^{4k} \rangle$. Find the coefficients in the perturbation expansion,

$$F(\lambda) = \sum_{k=0}^{\infty} C_k \, \lambda^k \, .$$

(c) Define the *remainder after* N terms as

$$R_N(\lambda) = F(\lambda) - \sum_{k=0}^N C_k \, \lambda^k \; .$$

Compute $R_N(\lambda)$ by evaluating numerically the integral for $F(\lambda)$ (using Mathematica or some other numerical package) and subtracting the finite sum. Then define the ratio $S_N(\lambda) = R_N(\lambda)/F(\lambda)$, which is the relative error from the N term approximation and plot the absolute relative error $|S_N(\lambda)|$ versus N for several values of λ . (I suggest you plot the error on a log scale.) What do you find?? Try a few values of λ including $\lambda = 0.01$, $\lambda = 0.05$, $\lambda = 0.2$, $\lambda = 0.5$, $\lambda = 1$, $\lambda = 2$.

(d) Repeat the calculation for the integral

$$G(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{1}{2} \, x^2 - \frac{\lambda}{6!} \, x^6\right) \,.$$

(e) Reflect meaningfully on the consequences for weakly and strongly coupled quantum field theories.

²⁶In fact, it does. According to Mathematica, $F(\lambda) = \sqrt{\frac{2u}{\pi}} \exp(u) K_{1/4}(u)$, where $u = 3/4\lambda$ and $K_{\nu}(z)$ is the modified Bessel function. I am grateful to Prof. John McGreevy for pointing this out.

Solution

(a) Clearly $\langle x^n \rangle = (d^n Z/dj^n) |_{j=0}$, and so $\langle x^n \rangle = (d^n Z/dj^n)_{j=0}$. With $Z(j) = \exp(\frac{1}{2}j^2)$, only the k^{th} order term in j^2 in the Taylor series for Z(j) contributes, and we obtain

$$\langle x^{2k} \rangle = \frac{d^{2k}}{dj^{2k}} \left(\frac{j^{2k}}{2^k k!} \right) = \frac{(2k)!}{2^k k!}$$

(b) We have

$$F(\lambda) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\lambda}{4!} \right)^n \langle x^{4n} \rangle = \sum_{n=0}^{\infty} \frac{(4n)!}{4^n (4!)^n n! (2n)!} (-\lambda)^n .$$

This series is *asymptotic*. It has the properties

$$\lim_{\lambda \to 0} \frac{R_N(\lambda)}{\lambda^N} = 0 \quad \text{(fixed } N\text{)} \qquad , \qquad \lim_{N \to \infty} \frac{R_N(\lambda)}{\lambda^N} = \infty \quad \text{(fixed } \lambda\text{)} ,$$

where $R_N(\lambda)$ is the remainder after *N* terms, defined in part (c). The radius of convergence is zero. To see this, note that if we reverse the sign of λ , then the integrand of $F(\lambda)$ diverges badly as $x \to \pm \infty$. So $F(\lambda)$ is infinite for $\lambda < 0$, which means that there is no disk of any finite radius of convergence which encloses the point $\lambda = 0$. Note that by Stirling's rule,

$$C_n \equiv \frac{(-1)^n \, (4n)!}{4^n \, (4!)^n \, n! \, (2n)!} \sim (-1)^n \, n^n \cdot \left(\frac{2}{3}\right)^n e^{-n} \cdot (\pi n)^{-1/2} \, ,$$

and we conclude that the magnitude of the summand reaches a minimum value when $n = n^*(\lambda)$, with $n^*(\lambda) \approx 3/2\lambda$ for small values of λ . For large n, the magnitude of the coefficient C_n grows as $|C_n| \sim e^{n \ln n + O(n)}$, which dominates the λ^n term, no matter how small λ is.

(c) Results are plotted in fig. 1.16.

It is worth pointing out that the series for $F(\lambda)$ and for $\ln F(\lambda)$ have diagrammatic interpretations. For a Gaussian integral, one has

$$\langle x^{2k} \rangle = \langle x^2 \rangle^k \cdot A_{2k}$$

where A_{2k} is the *number of contractions*. For our integral, $\langle x^2 \rangle = 1$. The number of contractions A_{2k} is computed in the following way. For each of the 2k powers of x, we assign an index running from 1 to 2k. The indices are *contracted*, *i.e.* paired, with each other. How many pairings are there? Suppose we start with any from among the 2k indices. Then there are (2k-1) choices for its mate. We then choose another index arbitrarily. There are now (2k-3) choices for *its* mate. Carrying this out to its completion, we find that the number of contractions is

$$A_{2k} = (2k-1)(2k-3)\cdots 3\cdot 1 = \frac{(2k)!}{2^k k!},$$



Figure 1.16: Relative error *versus* number of terms kept for the asymptotic series for $F(\lambda)$ (quartic theory). Note that the optimal number of terms to sum is $N^*(\lambda) \approx \frac{3}{2\lambda}$.

exactly as we found in part (a). Now consider the integral $F(\lambda)$. If we expand the quartic term in a power series, then each power of λ brings an additional four powers of x. It is therefore convenient to represent each such quartet with the symbol \times . At order N of the series expansion, we have $N \times s$ and 4N indices to contract. Each full contraction of the indices may be represented as a labeled diagram, which is in general composed of several disjoint connected subdiagrams. Let us label these subdiagrams, which we will call clusters, by an index γ . Now suppose we have a diagram consisting of m_{γ} subdiagrams of type γ , for each γ . If the cluster γ contains n_{γ} vertices (\times), then we must have

$$N = \sum_{\gamma} m_{\gamma} \, n_{\gamma} \, .$$

How many ways are there of assigning the labels to such a diagram? One might think $(4!)^N \cdot N!$, since for each vertex × there are 4! permutations of its four labels, and there are N! ways to permute all the vertices. However, this overcounts diagrams which are *invariant* under one or more of these permutations. We define the *symmetry factor* s_{γ} of the (unlabeled) cluster γ as the number of permutations of the indices of a corresponding labeled cluster which result in the same contraction. We can also permute the m_{γ} identical disjoint clusters of type γ .

Examples of clusters and their corresponding symmetry factors are provided in fig. 1.17, for all diagrams with $n_{\gamma} \leq 3$. There is only one diagram with $n_{\gamma} = 1$, resembling (•). To obtain $s_{\gamma} = 8$, note that each of the circles can be separately rotated by an angle π about the long symmetry axis. In addition, the figure can undergo a planar rotation by π about an axis which runs



Figure 1.17: Cluster symmetry factors for the quartic theory. A vertex is represented as a black dot (•) with four 'legs'.

through the sole vertex and is normal to the plane of the diagram. This results in $s_{\gamma} = 2 \cdot 2 \cdot 2 = 8$. For the cluster \bigcirc , there is one extra circle, so $s_{\gamma} = 2^4 = 16$. The third diagram in figure shows two vertices connected by four lines. Any of the 4! permutations of these lines results in the same diagram. In addition, we may reflect about the vertical symmetry axis, interchanging the vertices, to obtain another symmetry operation. Thus $s_{\gamma} = 2 \cdot 4! = 48$. One might ask why we don't also count the planar rotation by π as a symmetry operation. The answer is that it is equivalent to a combination of a reflection and a permutation, so it is not in fact a distinct symmetry operation. (If it were distinct, then s_{γ} would be 96.) Finally, consider the last diagram in the figure, which resembles a sausage with three links joined at the ends into a circle. If we keep the vertices fixed, there are 8 symmetry operations associated with the freedom to exchange the two lines associated with each of the three sausages. There are an additional 6 symmetry operations by $0, \frac{2\pi}{3}$ and $\frac{4\pi}{3}$, each of which can also be combined with a reflection about the *y*-axis (this is known as the group C_{3v}). Thus, $s_{\gamma} = 8 \cdot 6 = 48$.

Now let us compute an expression for $F(\gamma)$ in terms of the clusters. We sum over all possible numbers of clusters at each order:

$$F(\gamma) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\{m_{\gamma}\}} \frac{(4!)^N N!}{\prod_{\gamma} s_{\gamma}^{m_{\gamma}} m_{\gamma}!} \left(-\frac{\lambda}{4!}\right)^N \delta_{N,\sum_{\gamma} m_{\gamma} n_{\gamma}} = \exp\left(\sum_{\gamma} \frac{(-\lambda)^{n_{\gamma}}}{s_{\gamma}}\right).$$
(1.173)

Thus,

$$\ln F(\gamma) = \sum_{\gamma} \frac{(-\lambda)^{n_{\gamma}}}{s_{\gamma}} ,$$

and *the logarithm of the sum over all diagrams is a sum over connected clusters*. It is instructive to work this out to order λ^2 . We have, from the results of part (b),

$$F(\lambda) = 1 - \frac{1}{8}\lambda + \frac{35}{384}\lambda^2 + \mathcal{O}(\lambda^3) \implies \ln F(\lambda) = -\frac{1}{8}\lambda + \frac{1}{12}\lambda^2 + \mathcal{O}(\lambda^3).$$

λ	10	2	0.5	0.2	0.1	0.05	0.02
F	0.92344230	0.97298847	0.99119383	0.996153156	0.99800488	0.99898172	0.99958723
n^*	0.68	1.3	2.6	4.1	5.8	8.2	13

Table 1.1: $F(\lambda)$ and $n^*(\lambda)$ for part d.

Note that there is one diagram with N = 1 vertex, with symmetry factor s = 8. For N = 2 vertices, there are two diagrams, one with s = 16 and one with s = 48 (see fig. 1.17). Since $\frac{1}{16} + \frac{1}{48} = \frac{1}{12}$, the diagrammatic expansion is verified to order λ^2 .

(d) We now have²⁷

$$G(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{1}{2}x^2 - \frac{\lambda}{6!}x^6\right) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\lambda}{6!}\right)^n \langle x^{6n} \rangle \equiv \sum_{n=0}^{\infty} C_n \,\lambda^n \,, \tag{1.174}$$

with

$$C_n = \frac{(-1)^n \, (6n)!}{(6!)^n \, n! \, 2^{3n} \, (3n)!}$$

Invoking Stirling's approximation, we find $\ln |C_n| \sim 2n \ln n - (2 + \ln \frac{5}{3}) n$. Thus we see that the magnitude of the contribution of the n^{th} term in the perturbation series is given by

$$C_n \lambda^n = (-1)^n \exp\left(2n \ln n - \left(2 + \ln \frac{10}{3}\right)n + n \ln \lambda\right).$$

Differentiating, we find that this contribution is minimized for $n = n^*(\lambda) = (10/3\lambda)^{1/2}$. Via numerical integration using FORTRAN subroutines from QUADPACK, one obtains the results in Fig. 1.18 and Tab. 1.1.

The series for $G(\lambda)$ and for $\ln G(\lambda)$ again have diagrammatic interpretations. If we expand the sextic term in a power series, each power of λ brings an additional six powers of x. It is natural to represent each such sextet with as a vertex with six legs. At order N of the series expansion, we have N such vertices and 6N legs to contract. As before, each full contraction of the leg indices may be represented as a labeled diagram, which is in general composed of several disjoint connected clusters. If the cluster γ contains n_{γ} vertices, then for any diagram we again must have $N = \sum_{\gamma} m_{\gamma} n_{\gamma}$, where m_{γ} is the number of times the cluster γ appears. As with the quartic example, the number of ways of assigning labels to a given diagram is given by the total number of possible permutations $(6!)^N \cdot N!$ divided by a correction factor $\prod_{\gamma} s_{\gamma}^{m_{\gamma}} m_{\gamma}!$, where s_{γ} is the symmetry factor of the cluster γ , and the $m_{\gamma}!$ term accounts for the possibility of permuting among different labeled clusters of the same type γ .

²⁷According to Mathematica, the $G(\lambda)$ has the analytic form $G(\lambda) = \pi \sqrt{u} \left[\operatorname{Ai}^2(u) + \operatorname{Bi}^2(u) \right]$, where $u = (15/2\lambda)^{1/3}$ and $\operatorname{Ai}(z)$ and $\operatorname{Bi}(z)$ are Airy functions. The definitions and properties of the Airy functions are discussed in §9.2 of the NIST Handbook of Mathematical Functions.



Figure 1.18: Logarithm of ratio of remainder after *N* terms $R_N(\lambda)$ to the value of the integral $G(\lambda)$ for the sextic theory, for various values of λ .

Examples of clusters and their corresponding symmetry factors are provided in Fig. 1.19. There is only one diagram with $n_{\gamma} = 1$, shown panel (a), resembling a three-petaled flower. To obtain $s_{\gamma} = 48$, note that each of the petals can be rotated by 180° about an axis bisecting the petal, yielding a factor of 2^3 . The three petals can then be permuted, yielding an additional factor of 3!. Hence the total symmetry factor is $s_{\gamma} = 2^3 \cdot 3! = 48$. Now we can see how dividing by the symmetry factor saves us from overcounting. In this case, we get $6!/s_{\gamma} = 720/48 = 15 = 5 \cdot 3 \cdot 1$, which is the correct number of contractions. For the diagram in panel (b), the four petals and the central loop can each be rotated about a symmetry axis, yielding a factor 2^5 . The two left petals can be permuted, as can the two right petals. Finally, the two vertices can themselves be permuted. Thus, the symmetry factor is $s_{\gamma} = 2^5 \cdot 2^2 \cdot 2 = 2^8 = 256$. In panel (c), the six lines can be permuted (6!) and the vertices can be exchanged (2), hence $s_{\gamma} = 6! \cdot 2 = 1440$. In panel (d), the two outer loops each can be twisted by 180° , the central four lines can be permuted, and the vertices can be permuted, hence $s_{\gamma} = 2^2 \cdot 4! \cdot 2 = 192$. Finally, in panel (e), each pair of vertices is connected by three lines which can be permuted, and the vertices themselves can be permuted, so $s_{\gamma} = (3!)^3 \cdot 3! = 1296$.

Now let us compute an expression for $F(\gamma)$ in terms of the clusters. We sum over all possible numbers of clusters at each order:

$$G(\gamma) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\{m_{\gamma}\}} \frac{(6!)^{N} N!}{\prod_{\gamma} s_{\gamma}^{m_{\gamma}} m_{\gamma}!} \left(-\frac{\lambda}{6!}\right)^{N} \delta_{N, \sum_{\gamma} m_{\gamma} n_{\gamma}} = \exp\left(\sum_{\gamma} \frac{(-\lambda)^{n_{\gamma}}}{s_{\gamma}}\right).$$
(1.175)



Figure 1.19: Diagrams and their symmetry factors for the $\frac{1}{6!}\lambda x^6$ zero-dimensional field theory.

Thus,

$$\ln G(\gamma) = \sum_{\gamma} \frac{(-\lambda)^{n_{\gamma}}}{s_{\gamma}}$$

and *the logarithm of the sum over all diagrams is a sum over connected clusters*. It is instructive to work this out to order λ^2 . We have, from the results of part (a),

$$G(\lambda) = 1 - \frac{\lambda}{2^6 \cdot 3} + \frac{7 \cdot 11 \cdot \lambda^2}{2^9 \cdot 3 \cdot 5} + \mathcal{O}(\lambda^3) \implies \ln G(\lambda) = -\frac{\lambda}{2^6 \cdot 3} + \frac{113 \cdot \lambda^2}{2^8 \cdot 3^2 \cdot 5} + \mathcal{O}(\lambda^3)$$

Note that there is one diagram with N = 1 vertex, with symmetry factor s = 48. For N = 2 vertices, there are three diagrams, one with s = 256, one with s = 1440, and one with s = 192 (see Fig. 1.19). Since $\frac{1}{256} + \frac{1}{1440} + \frac{1}{192} = \frac{113}{2^83^25}$, the diagrammatic expansion is verified to order λ^2 .

(e) In quantum field theory (QFT), the vertices themselves carry space-time labels, and the contractions, *i.e.* the lines connecting the legs of the vertices, are *propagators* $G(x_i^{\mu} - x_j^{\mu})$, where x_i^{μ} is the space-time label associated with vertex *i*. It is convenient to work in momentum-frequency space, in which case we work with the Fourier transform $\hat{G}(p^{\mu})$ of the space-time propagators. Integrating over the space-time coordinates of each vertex then enforces total 4-momentum conservation at each vertex. We then must integrate over all the internal 4-momenta to obtain the numerical value for a given diagram. The diagrams, as you know, are associated with Feynman's approach to QFT and are known as Feynman diagrams. Our example here is equivalent to a (0+0)-dimensional field theory, *i.e.* zero space dimensions and zero time dimensions. There are then no internal 4-momenta to integrate over, and each propagator is simply a number rather than a function. The discussion above of symmetry factors s_{γ} carries over to the more general QFT case. There is an important lesson to be learned here about the behavior of asymptotic series. As we have seen, if λ is sufficiently small, summing more and more terms in the perturbation series results in better and better results, until one reaches an optimal order when the error is minimized. Beyond this point, summing additional terms makes the result *worse*, and indeed the perturbation series diverges badly as $N \to \infty$. Typically the optimal order of perturbation theory is inversely proportional to the coupling constant. For quantum electrodynamics (QED), where the coupling constant is the fine structure constant $\alpha = e^2/\hbar c \approx \frac{1}{137}$, we lose the ability to calculate in a reasonable time long before we get to 137 loops, so practically speaking no problems arise from the lack of convergence. In quantum chromodynamics (QCD), however, the effective coupling constant is about two orders of magnitude larger, and perturbation theory is a much more subtle affair.

1.9 Appendix : Derivation of Ginzburg-Landau Functional

1.9.1 Discrete symmetry : \mathbb{Z}_2

We start with the Ising Hamiltonian,

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} \,\sigma_i \,\sigma_j - \sum_i h_i \,\sigma_i + \frac{1}{2} \sum_i J_{ii} \quad , \qquad (1.176)$$

where $\sigma_i \in \{+1, -1\}$ for all *i*. By subtracting the last term, we eliminate the constant contribution from the diagonal elements of the coupling matrix J_{ij} . You might well wonder why we simply don't specify that $J_{ii} = 0$ for all *i* from the outset. The reason for this will be made apparent at an important moment, and the suspense should motivate you to read further!

We define $K_{ij} \equiv J_{ij}/k_{\rm B}T$ and $g_i \equiv h_i/k_{\rm B}T$, so the density matrix is²⁸

$$\varrho(\boldsymbol{\sigma}) = \exp\left(\frac{1}{2}K_{ij}\,\sigma_i\,\sigma_j + g_i\,\sigma_i - \frac{1}{2}\,\mathsf{Tr}\,K\right) \quad . \tag{1.177}$$

We now invoke the following identity:

$$\int_{-\infty}^{\infty} dm_1 \cdots \int_{-\infty}^{\infty} dm_N \, \exp\left[-\frac{1}{2} K_{ij}^{-1} m_i \, m_j + b_i \, m_i\right] = (2\pi \det K)^{1/2} \exp\left[\frac{1}{2} K_{ij} \, b_i \, b_j\right] \quad . \tag{1.178}$$

This licenses us to write

$$\varrho(\boldsymbol{\sigma}) = (2\pi \det K)^{-1/2} e^{-\frac{1}{2}\operatorname{Tr} K} \int d^N m \exp\left[-\frac{1}{2}K_{ij}^{-1}m_im_j + (m_i + g_i)\sigma_j\right] \quad .$$
(1.179)

²⁸In fact what we call $\rho(\sigma)$ is really the diagonal element $\rho(\sigma | \sigma) = \langle \sigma | \rho | \sigma \rangle$ of the density matrix, whose off-diagonal matrix elements all vanish since all operators σ_i commute for our noninteracting Hamiltonian.

Now trace over the $\{\sigma_i\}$ to obtain the partition function:

$$Z = \int d^{N}m \, \exp\left[-\Phi(\boldsymbol{m})\right] \quad , \tag{1.180}$$

where

$$\Phi(\boldsymbol{m}) = \Phi_0 + \frac{1}{2} \sum_{i,j} K_{ij}^{-1} m_i m_j - \sum_i \ln\left[\cosh(m_i + g_i)\right] \quad , \tag{1.181}$$

where $\Phi_0 = \frac{1}{2} \ln(2\pi \det K) + \frac{1}{2} \operatorname{Tr} K - N \ln 2$. Note also that $\langle \sigma_i \rangle = \langle \tanh(m_i + g_i) \rangle$.

We consider the situation where we are close to a second order phase transition and we apply a very weak field. In this case, we may expand $\Phi(\mathbf{m})$ in powers of the m_i and g_i to obtain

$$\Phi(\boldsymbol{m}) = \Phi_0 + \frac{1}{2} K_{ij}^{-1} m_i m_j + \sum_i \left(-g_i m_i - \frac{1}{2} m_i^2 + \frac{1}{12} m_i^4 + \dots \right) \quad , \tag{1.182}$$

valid to fourth order in the $\{\phi_i\}$ and first order in the $\{g_i\}$. Now define the Fourier transforms,

$$m_i = \frac{1}{\sqrt{N}} \sum_{k} \hat{m}_k e^{-k \cdot R_i} , \qquad \hat{m}_k = \frac{1}{\sqrt{N}} \sum_{i} m_i e^{-ik \cdot R_i}$$
(1.183)

as well as $\hat{K}(k) \equiv \sum_{R} K(R) e^{-ik \cdot R}$, with $K_{ij} = K(R_j - R_i)$. We obtain

$$\Phi(\boldsymbol{m}) = \Phi_0 + \frac{1}{2} \sum_{\boldsymbol{k}} \left(\hat{K}^{-1}(\boldsymbol{k}) - 1 \right) |\hat{m}_{\boldsymbol{k}}|^2 + \frac{1}{12} \sum_{i} m_i^4 - \sum_{i} g_i m_i \quad , \qquad (1.184)$$

where $\hat{K}^{-1}(\mathbf{k}) = 1/\hat{K}(\mathbf{k})$. On a *d*-dimensional cubic lattice with lattice constant *a*, assuming J_{ij} has isotropic nearest neighbor interactions only, we have

$$\hat{K}(\mathbf{k}) = 2K \sum_{\mu=1}^{d} \cos(k_{\mu}a) = 2dK - K\mathbf{k}^{2}a^{2} + \mathcal{O}(k_{\mu}^{4}) \quad , \tag{1.185}$$

where $K = J/k_{\rm B}T$ and J is the nearest neighbor coupling. One might think we could simply expand about the global maximum of $\hat{K}(\mathbf{k})$ lying at $\mathbf{k} = \mathbf{0}$ and then invert, to obtain

$$\hat{K}(\mathbf{k}) \approx \frac{1}{2dK} + \frac{1}{4d^2K} \, \mathbf{k}^2 a^2 + \dots$$
 (1.186)

In the absence of an external field, the coefficient of the quadratic term in each m_i would then be $\frac{1}{2}\alpha$ with Landau parameter $\alpha = (2dK)^{-1} - 1$. This would predict an ordered phase for a < 0, or $k_{\rm B}T < zJ$, where z = 2d is the lattice coordination number, which is indeed the classic mean field theory result.

However, there is a disturbing aspect to our derivation, which thus far has been exact. The determinant of *K* is given by det $K = \prod_{k} \hat{K}(k)$, and this vanishes when any of the eigenvalues

 $K(\mathbf{k})$ vanishes. It is easy to conjure up a vanishing eigenvalue, for example by taking $k_{\mu} = \pi/2a$ for all $\mu \in \{1, \ldots, d\}$. Indeed, the eigenspectrum of K extends over the interval $\hat{K}(\mathbf{k}) \in [-2dK, +2dK]$, hence there are negative eigenvalues as well. We can escape this problem by noting that our formulation allows us to include *arbitrary* diagonal elements in the matrix K. They are guaranteed not to affect our final result – if it is obtained exactly – since each diagonal element J_{ii} cancels in the expression for H in Eqn. 1.201. Thus, we may take

$$J_{ij} = J_0 + J_1 \,\delta_{|\mathbf{R}_i - \mathbf{R}_j|,a} \quad , \tag{1.187}$$

which yields

$$\hat{K}(\mathbf{k}) = K_0 + 2K_1 \sum_{\mu=1}^d \cos(k_\mu a) = K_0 + 2dK_1 - K_1 \mathbf{k}^2 a^2 + \dots \quad .$$
(1.188)

Provided $K_0 > 2dK_1$, all the eigenvalues $\hat{K}(\mathbf{k})$ are positive, and we may safely expand about $\mathbf{k} = \mathbf{0}$, obtaining

$$\hat{K}^{-1}(\mathbf{k}) = \frac{k_{\rm B}T}{J_0 + zJ_1} \left(1 + \frac{J_1}{J_0 + zJ_1} \, \mathbf{k}^2 a^2 + \dots \right) \quad . \tag{1.189}$$

The low temperature phase occurs for $\hat{K}(\mathbf{0}) < 1$, which means $k_{\rm B}T < J_0 + zJ_1$. Thus we have $k_{\rm B}T_{\rm c} = J_0 + zJ_1$, which unfortunately depends on the (almost²⁹) arbitrary constant J_0 . This is perhaps unsatisfying, since adding J_0 increases $T_{\rm c}$, and mean field theory already tends to overestimate the critical temperature. However, we shouldn't be too alarmed by any of this. We have no right to trust in low order expansions when it comes to predicting $T_{\rm c}$. However, from the standpoint of the renormalization group, we may expect the corresponding continuum field theory, with free energy

$$F[m] = \int d^d x \left(\frac{1}{2} a m^2 + \frac{1}{4} b m^4 + \frac{1}{2} \kappa |\nabla m|^2 - hm \right) \quad , \tag{1.190}$$

to yield the correct critical exponents.

The Euler-Lagrange equations derived from the free energy in Eqn. 1.190 are

$$a m + b m^3 - \kappa \nabla^2 m = h \quad . \tag{1.191}$$

Consider the case a < 0 and h = 0, in which case the lowest free energy solution corresponds to $m(\mathbf{x}) = \pm m_0$ with $m_0 = \sqrt{|a|/b}$, and write $m(\mathbf{x}) = m_0 \mu(\mathbf{x})$. Let's solve for the case of a domain wall, where $\mu(\mathbf{x}) = \mu(x_1)$ is a function of only one coordinate and interpolates between the two vacuua, with $\mu(-\infty) = -1$ and $\mu(+\infty) = +1$. We then have

$$\xi^2 \frac{d^2 \mu}{dx_1^2} = -\mu + \mu^3 = -\frac{dU}{d\mu}$$
(1.192)

²⁹Recall $J_0 > 2dJ_1$ must be imposed in order to avoid a vanishing of the determinant det K.

where $\xi = \sqrt{\kappa/|a|}$ is the correlation length, and

$$U(\mu) = -\frac{1}{4} \left(1 - \mu^2\right)^2 \quad . \tag{1.193}$$

Thus, we have

$$2\xi \frac{d\mu}{dx_1} = 1 - \mu^2 \quad , \tag{1.194}$$

with solution

$$\mu(x_1) = \tanh(x_1/2\xi) \quad , \tag{1.195}$$

which satisfies the boundary conditions $\mu(\pm \infty) = \pm 1$. Thus, our domain wall profile is given by the expression $m(x) = m_0 \tanh(x_1/2\xi)$, and the total domain wall energy is found to be

$$\Delta F = \frac{a^2}{2b} L^{d-1} \int_{-\infty}^{\infty} dx_1 \left\{ \frac{1}{2} \left(1 - \mu^2\right)^2 + \left(\xi \frac{d\mu}{dx_1}\right)^2 \right\} = \frac{4a^2}{b} \xi L^{d-1} \quad , \tag{1.196}$$

which has the same *L* dependence as what we found in $\S1.5.1$ for the Ising case.

1.9.2 Continuous symmetry : O(n)

A general *n*-dimensional unit vector $\phi = (\phi^1, \dots, \phi^n)$ may be expressed in terms of n - 2 polar angles $\{\theta_1, \dots, \theta_{n-2}\}$ and one azimuthal angle φ , *viz*.

$$\begin{aligned}
\phi^{1} &= \sin \theta_{1} \cdots \sin \theta_{n-3} \sin \theta_{n-2} \cos \varphi \\
\phi^{2} &= \sin \theta_{1} \cdots \sin \theta_{n-3} \sin \theta_{n-2} \sin \varphi \\
\phi^{3} &= \sin \theta_{1} \cdots \sin \theta_{n-3} \cos \theta_{n-2} \\
&\vdots \\
\phi^{n-1} &= \sin \theta_{1} \cos \theta_{2} \\
\phi^{n} &= \cos \theta_{1} \quad .
\end{aligned}$$
(1.197)

Here $\theta_j \in [0, \pi]$ with $j \in \{1, ..., n-2\}$ and $\varphi \in [0, 2\pi]$. The total solid angle in n dimensions is then

$$\Omega_n = 2\pi \int_0^{\pi} d\theta_1 \cdots \int_0^{\pi} d\theta_{n-2} \sin^{n-2} \theta_1 \cdots \sin \theta_{n-2}$$
(1.198)

Now

$$\int_{0}^{\pi} d\theta \, \sin^{p}\theta = \frac{\sqrt{\pi} \, \Gamma(\frac{p+1}{2})}{\Gamma(\frac{p+2}{2})} \quad , \tag{1.199}$$

and therefore

$$\Omega_n = 2\pi \cdot \frac{\sqrt{\pi} \,\Gamma(\frac{n-1}{2})}{\Gamma(\frac{n}{2})} \cdot \frac{\sqrt{\pi} \,\Gamma(\frac{n-2}{2})}{\Gamma(\frac{n-1}{2})} \cdots \frac{\sqrt{\pi} \,\Gamma(1)}{\Gamma(\frac{3}{2})} = \frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})} \quad . \tag{1.200}$$

This agrees with the following method of calculation:

$$\pi^{n/2} = \left(\int_{-\infty}^{\infty} dx \, e^{-x^2}\right)^n = \int d^n r \, e^{-r^2} = \Omega_n \int_0^{\infty} dr \, r^{n-1} \, e^{-r^2} = \frac{1}{2} \Omega_n \int_0^{\infty} du \, u^{\frac{n}{2}-1} \, e^{-u} = \frac{1}{2} \Omega_n \, \Gamma(\frac{n}{2}) \quad .$$

Consider now the O(n) model Hamiltonian,

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} \,\hat{\phi}_i \cdot \hat{\phi}_j - \sum_i h_i \cdot \hat{\phi}_i + \frac{1}{2} \sum_i J_{ii} \quad , \qquad (1.201)$$

Using the Gaussian integral identity of Eqn. 1.178 *n* times, we obtain

$$Z = \int d^{n}m_{1} \cdots \int d^{n}m_{N} \exp\left[-\Phi(\boldsymbol{m}_{1},\ldots,\boldsymbol{m}_{N})\right]$$
(1.202)

where each $m_i = (m_i^1, \dots, m_i^n)$ is a real valued *n*-component vector, and

$$\Phi(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n) = \Phi_0 + \frac{1}{2} \sum_{i,j} K_{ij} \, \boldsymbol{m}_i \cdot \boldsymbol{m}_j - \sum_i \ln Y_n \big(|\boldsymbol{m}_i + \boldsymbol{g}_i| \big) \quad , \tag{1.203}$$

with $\Phi_0=\frac{n}{2}\ln(2\pi\det K)+\frac{1}{2}\operatorname{Tr} K$, $\boldsymbol{g}_i=\boldsymbol{h}_i/k_{\scriptscriptstyle \mathrm{B}}T$, and

$$Y_{n}(y) = \ln\left(\int_{0}^{\pi} d\theta \,\left[\sin\theta\right]^{n-2} e^{y\cos\theta} \middle/ \int_{0}^{\pi} d\theta \,\left[\sin\theta\right]^{n-2}\right) = \frac{y^{2}}{2n} - \frac{y^{4}}{8n^{2}(n+1)} + \mathcal{O}(y^{6}) \quad . \quad (1.204)$$

Expanding to linear order in the fields $\{g_i\}$ and quadratic order in the local order parameter values $\{m_i\}$, we obtain

$$\Phi(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_N) = \Phi_0 + \frac{1}{2} \sum_{\boldsymbol{k}} \left(\hat{K}^{-1}(\boldsymbol{k}) - \frac{1}{n} \right) |\hat{\boldsymbol{m}}_{\boldsymbol{k}}|^2 + \sum_{i} \frac{|\boldsymbol{m}_i|^4}{8n^2(n+1)} - \frac{1}{N} \sum_{i} \boldsymbol{g}_i \cdot \boldsymbol{m}_i + \dots$$
(1.205)

which, in the continuum limit, corresponds to the dimensionless free energy density

$$\beta f(\boldsymbol{m}, \boldsymbol{\nabla} \boldsymbol{m}) = f_0 + \frac{1}{2} a(T) \, \boldsymbol{m}^2 + \frac{1}{4} \, b \, (\boldsymbol{m}^2)^2 + \frac{1}{2} \, \kappa \, (\boldsymbol{\nabla} \boldsymbol{m})^2 - \boldsymbol{j} \cdot \boldsymbol{m} + \dots \quad . \tag{1.206}$$

Assuming a(T) < 0, we find the equilibrium value $|\mathbf{m}| = m_0 = \sqrt{|a|/b}$. Writing $\mathbf{m} = m_0 \hat{\boldsymbol{\omega}}$, where $\hat{\boldsymbol{\omega}}(\mathbf{x})$ is a unit vector field, and setting the external field to $\mathbf{j} = 0$, we find the free energy density for twists of the direction vector $\hat{\boldsymbol{\omega}}$ to be

$$f_{\text{twist}}(\hat{\boldsymbol{\omega}}) = \frac{1}{2} \rho_{\text{s}} \left(\boldsymbol{\nabla} \hat{\boldsymbol{\omega}} \right)^2 \quad , \tag{1.207}$$

where the *spin stiffness* is $\rho_s = \kappa m_0^2 k_B T$, which has dimensions EL^{2-d} . As shown in §1.5.1, a full twist in $\hat{\omega}(\boldsymbol{x})$ in a single plane (ω^1, ω^2) across the width L of the system yields an energy which is proportional to L^{d-2} .