8.334 Statistical Mechanics II: Statistical Physics of Fields
Spring 2008

I. Collective Behavior, From Particles to Fields

I.A Introduction

The object of the first part of this course was to introduce the principles of statistical mechanics which provide a bridge between the fundamental laws of microscopic physics, and observed phenomena at macroscopic scales.

Microscopic Physics is characterized by large numbers of degrees of freedom; for example, the set of positions and momenta $\{\vec{p}_i, \vec{q}_i\}$, of particles in a gas, configurations of spins $\{\vec{s}_i\}$, in a magnet, or occupation numbers $\{n_i\}$, in a grand canonical ensemble. The evolution of these degrees of freedom is governed by an underlying Hamiltonian $\mathcal{H}$.

Macroscopic Physics is usually described by a few equilibrium state variables such as pressure P, volume V, temperature T, internal energy E, entropy S, etc., which obey the laws of thermodynamics.

Statistical Mechanics provides a probabilistic connection between the two realms. For example, in a canonical ensemble of temperature T, each micro-state μ, of the system occurs with a probability $p(\mu) = \exp\left(-\beta\mathcal{H}(\mu)\right)/Z$, where $\beta = (k_B T)^{-1}$. To insure that the total probability is normalized to unity, the *partition function $Z(T)$* must equal $\sum_\mu \exp\left(-\beta\mathcal{H}(\mu)\right)$. Thermodynamic information about the *macroscopic* state of the system is then extracted from the *free energy $F = -k_B T \ln Z$*.

The above program can in fact be fully carried out only for a limited number of simple systems; mostly describing non–interacting collections of particles where the partition function can be calculated exactly. Some effects of interactions can be included by perturbative treatments around such exact solutions. However, even for the relatively simple case of an imperfect gas, the perturbative approach breaks down close to the condensation point. One the other hand, it is precisely the multitude of new phases and prperties resulting from interactions that renders macroscopic physics interesting. In particular, we would like to address the following questions:

(1) In the thermodynamic limit ($N \to \infty$), strong interactions lead to new phases of matter. We studied the simplest example of the liquid gas transition in some detail, but there are in fact many other interesting phases such as solids, liquid–crystals, magnets, superconductors, etc. How can we describe the emergence of such distinct macroscopic behavior from the interactions of the underlying particles? What are the thermodynamic variables that describe the macroscopic state of these phases; and

what are their identifying signatures in measurements of bulk response functions (heat capacity, susceptibility, etc.)?

(2) What are the characteristic low energy excitations of the system? As in the case of phonons in solids or in superfluid helium, low energy excitations are typically *collective modes*, which involve the coordinated motions of many microscopic degrees of freedom (particles). These modes are easily excited by thermal fluctuations, and probed by scattering experiments.

The underlying microscopic Hamiltonian for the interactions of particles is usually quite complicated, making an *ab initio* particulate approach to the problem intractable. However, there are many common features in the macroscopic behavior of many such systems that can still be fruitfully studied by the methods of statistical mechanics. Although, the interactions between particles are very different at the microscopic scale, one may hope that averaging over sufficiently many particles leads to a simpler description. (In the same sense that the central limit theorem ensures that the sum over many random variables has a simple Gaussian distribution.) This expectation is indeed justified in many cases where the collective behavior of the interacting system becomes more simple at long wavelengths and long times. (This is sometimes called *hydrodynamic limit* by analogy to the Navier–Stokes equations for a fluid of particles.) The averaged variables appropriate to these length and time scales are no longer the discrete set of particle degrees of freedom, but slowly varying continuous *fields*. For example, the velocity field that appears in the Navier–Stokes equations is quite distinct from the velocities of the individual particles in the fluid. Hence the productive method for the study of collective behavior in interacting systems is the Statistical Mechanics of Fields. Thus the program of this course is,

• **Goal:** To learn to describe and classify states of matter, their collective properties, and the mechanisms for transforming from one phase to another.

• **Tools:** Methods of classical field theories; use of symmetries, treatment of nonlinearities by perturbation theory, and the renormalization group (RG) method.

• **Scope:** To provide sufficient familiarity with the material so that you can follow the current literature on such subjects as phase transitions, growth phenomena, polymers, superconductors, etc.

I.B Phonons and Elasticity

The theory of elasticity represents one of the simplest examples of a field theory. We shall demonstrate how certain properties of an elastic medium can be obtained, either by

the complicated method of starting from first principles, or by the much simpler means of appealing to symmetries of the problem. As such, it represents a prototype of how much can be learned from a phenomenological approach. The actual example has little to do with the topics that will be covered in this course, but it fully illustrates the methodology that will be employed. The problem of computing the low temperature heat capacity of a solid can be studied by both *ab initio* and *phenomenological* methods.

(i) *Ab initio* **(particulate) approach:** Calculating the heat capacity of a solid material from first principles is rather complicated. We breifly sketch some of the steps:

• The *ab initio* starting point is the Schrödinger equation for electrons and ions which can only be treated approximately, say by a density functional formalism. Instead, we start with a many body potential energy for the *ionic* coordinates $\mathcal{V}(\vec{q}_1, \vec{q}_2, \cdots, \vec{q}_N)$, which may itself be the outcome of such a quantum mechanical treatment.

• Ideal lattice positions at zero temperature are obtained by minimizing $\mathcal{V}$, typically forming a lattice $\vec{q}^*(\ell, m, n) = [\ell\hat{a} + m\hat{b} + n\hat{c}] \equiv \vec{q}^*_{\vec{r}}$, where $\vec{r} = \{\ell, m, n\}$ is a triplet of integers, and $\hat{a}$, $\hat{b}$, and $\hat{c}$ are unit vectors.

• Small fluctuations about the ideal positions (due to finite temperature or quantum effects) are included by setting $\vec{q}_{\vec{r}} = \vec{q}^*_{\vec{r}} + \vec{u}(\vec{r})$. The cost of deformations in the potential energy is given by

$$\mathcal{V} = \mathcal{V}^* + \frac{1}{2} \sum_{\substack{\vec{r}, \vec{r}' \\ \alpha, \beta}} \frac{\partial^2 \mathcal{V}}{\partial q_{\vec{r},\alpha} \partial q_{\vec{r}',\beta}} u_\alpha(\vec{r})\ u_\beta(\vec{r}') + O(u^3), \tag{I.1}$$

where the indices α and β denote spatial components. (Note that the first derivative of $\mathcal{V}$ vanishes at the equilibrium position.) The full Hamiltonian for small deformations is obtained by adding the kinetic energy $\sum_{\vec{r},\alpha} p_\alpha(\vec{r})^2/2m$ to eq.(I.1), where $p_\alpha(\vec{r})$ is the momentum conjugate to $u_\alpha(\vec{r})$.

• The next step is to find the normal modes of vibration (phonons) by diagonalizing the matrix of derivatives. Since the ground state configuration is a regular lattice, the elements of this matrix must satisfy various translation and rotation symmetries. For example, they can only depend on the difference between the position vectors of ions $\vec{r}$ and $\vec{r}'$, i.e.

$$\frac{\partial^2 \mathcal{V}}{\partial q_{\vec{r},\alpha} \partial q_{\vec{r}',\beta}} = K_{\alpha\beta}(\vec{r} - \vec{r}'). \tag{I.2}$$

3

This translational symmetry allows us to at least partially diagonalize the Hamiltonian by using the Fourier modes,

$$u_\alpha(\vec{r}) = {\sum_{\vec{k}}}' \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{N}} u_\alpha(\vec{k}). \tag{I.3}$$

(Only *wavevectors* $\vec{k}$ inside the first *Brillouin zone* contribute to the sum.) The Hamiltonian then reads

$$\mathcal{H} = \mathcal{V}^* + \frac{1}{2} \sum_{\vec{k},\alpha,\beta} \left[\frac{|p_\alpha(\vec{k})|^2}{m} + K_{\alpha\beta}(\vec{k}) u_\alpha(\vec{k}) u_\beta(\vec{k})^* \right]. \tag{I.4}$$

While the precise form of the Fourier transformed matrix $K_{\alpha\beta}(\vec{k})$ is determined by the microscopic interactions, it has to respect the underlying symmetries of the crystallographic point group. Let us assume that diagonalizing this 3×3 matrix yileds eigenvalues $\{\kappa_\alpha(k)\}$ The quadratic part of the Hamiltonian is now decomposed into a set of independent (non–interacting) harmonic oscillators.

- The final step is to quantize each oscillator, leading to

$$\mathcal{H} = \mathcal{V}^* + \sum_{\vec{k},\alpha} \hbar\omega_\alpha(\vec{k}) \left(n_\alpha(\vec{k}) + \frac{1}{2} \right), \tag{I.5}$$

where $\omega_\alpha(\vec{k}) = \sqrt{\kappa_\alpha(\vec{k})/m}$, and $\{n_\alpha(\vec{k})\}$ are the set of occupation numbers. The average energy at a temperature T is given by

$$E(T) = \mathcal{V}^* + \sum_{\vec{k},\alpha} \hbar\omega_\alpha(\vec{k}) \left(\left\langle n_\alpha(\vec{k}) \right\rangle + \frac{1}{2} \right), \tag{I.6}$$

where we know from elementary statistical mechanics that the average occupation numbers are given by $\langle n_\alpha(\vec{k}) \rangle = 1/\left(\exp(\frac{\hbar\omega_\alpha}{k_B T}) - 1 \right)$. Clearly $E(T)$, and other macroscopic functions, have a complex behavior, dependent upon microscopic details through $\{\kappa_\alpha(k)\}$. Are there any features of these functions (e.g. the functional dependence as $T \to 0$) that are independent of microscopic features? The answer is positive, and illustrated with a one dimensional example.
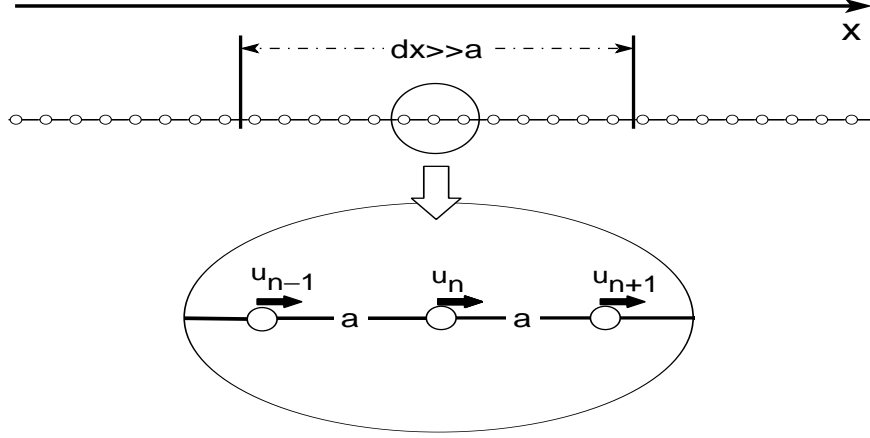
I.1. Displacements of a one–dimensional chain, and coarse–graining.

Consider a chain of particles, constrained to move in one dimension. A most general quadratic potential energy for deformations $\{u_n\}$, around an average separation of a, is

$$\mathcal{V} = \mathcal{V}^* + \frac{K_1}{2}\sum_n (u_{n+1} - u_n)^2 + \frac{K_2}{2}\sum_n (u_{n+2} - u_n)^2 + \cdots. \tag{I.7}$$

The decomposition to normal modes is obtained via

$$u_n = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} e^{-ikna} u(k), \quad \text{where} \quad u(k) = a\sum_n e^{ikna} u_n . \tag{I.8}$$

(Note the difference in normalizations from eq. (I.3).) The resulting potential energy is,

$$\mathcal{V} = \mathcal{V}^* + \frac{K_1}{2}\sum_n \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi}\frac{dk'}{2\pi}(e^{ika} - 1)(e^{ik'a} - 1)e^{-i(k+k')na} u(k)u(k') + \cdots. \tag{I.9}$$
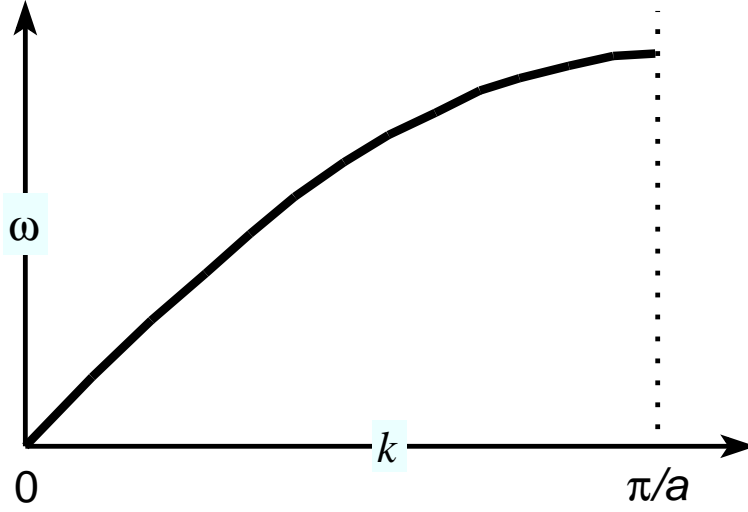
Using the identity $\sum_n e^{-i(k+k')na} = \delta(k + k')2\pi/a$, and noting that $u(-k) = u^*(k)$, we obtain

$$\mathcal{V} = \mathcal{V}^* + \frac{1}{2a}\int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi}\left[K_1(2 - 2\cos ka) + K_2(2 - 2\cos 2ka) + \cdots\right]|u(k)|^2. \tag{I.10}$$

The frequency of normal modes, given by $\omega(k) = \sqrt{[2K_1(1 - \cos ka) + \cdots]|/m}$, is depicted below. In the limit $k \to 0$, $\omega(k) \to v|k|$, where the 'sound velocity' v equals $a\sqrt{K/m}$ (see below).

The internal energy of these excitations, for a chain of N particles, is

$$E(T) = \mathcal{V}^* + Na\int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi}\frac{\hbar\omega(k)}{\exp\left(\hbar\omega(k)/k_B T\right) - 1}. \tag{I.11}$$

5

I.2. The dispersion of phonon modes for a linear chain.

As $T \to 0$, only modes with $\hbar\omega(k) < k_B T$ are excited. Hence only the $k \to 0$ part of the excitation spectrum is important and $E(T)$ simplifies to

$$E(T) = \mathcal{V}^* + Na \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\hbar v |k|}{\exp(\hbar v |k|/k_B T) - 1} = \mathcal{V}^* + Na \frac{\pi^2}{6\hbar v} (k_B T)^2. \qquad (\text{I.12})$$

Note:

(1) The full spectrum of excitation energies is

$$\frac{K(k)}{2} = K_1 (1 - \cos ka) + K_2 (1 - \cos 2ka) + \cdots \implies \frac{\bar{K}}{2} k^2 \quad \text{as} \quad k \to 0, \qquad (\text{I.13})$$

Further neighbor interactions change the speed of sound, but not the form of the dispersion relation as $k \to 0$.

(2) The heat capacity $C(T) = dE/dT$ is proportional to T. This dependence is a *universal* property, i.e. not material specific, and independent of the choice of the interatomic interactions.

(3) The T^2 dependence of energy comes from excitations with $k \to 0$ (or $\lambda \to \infty$), i.e. from collective modes involving many particles. These are precisely the modes for which statistical considerations may be meaningful.

(ii) Phenomenological (field) approach: We now outline a mesoscopic approach to the same problem, and show how it provides additional insights and is easily generalized to higher dimensions. Typical excitations at low temperatures have wavelengths $\lambda > \lambda(T) \approx (\hbar v / kT) \gg a$, where a is a lattice spacing. We can eliminate the unimportant short wavelength modes by an averaging process known as **coarse graining**. The idea is

6

consider a point x, and an interval $a \ll dx \ll \lambda(T)$ around it (Fig. I.1). In dx all the displacements u are approximately the same; and we can define an average deformation field $u(x)$. The kinetic energy is now related to the density $\rho = m/a$ via $\rho \int dx \dot{u}(x)^2/2$. Note that $u(x)$ is treated as a continuous function, but it certainly does not have any variations over distances smaller than the lattice spacing a.

What is the most general potential energy functional $\mathcal{V}[u]$, for the chain? A priori, we don't know much about the form of $\mathcal{V}[u]$, but we can construct it using the following general principles:

Locality: In most situations, the interactions between particles are short range, allowing us to define a potential energy *density* Φ at each point x, with $\mathcal{V}[u] = \int dx \Phi\big(u(x), du/dx, \cdots\big)$. Naturally, by including all derivatives we can also describe long-range interactions. In this context, the term *locality* implies that the higher derivative terms are less significant.

Translational symmetry: A uniform translation of the chain does not change its internal energy, and hence the energy density must satisfy the constraint $\Phi[u(x) + c] = \Phi[u(x)]$. This implies that Φ cannot depend directly on $u(x)$, but only on its derivatives du/dx, $d^2u/dx^2, \cdots$.

Stability: Since the fluctuations are around the *equilibrium* solution, there can be no linear terms in u or its derivatives. (Stability further requires that the quadratic part of $\mathcal{V}[u]$ must be positive definite.)

The most general potential consistent with these constraints is

$$\mathcal{V}[u] = \int dx \left[\frac{K}{2} \left(\frac{\partial u}{\partial x} \right)^2 + \frac{L}{2} \left(\frac{\partial^2 u}{\partial^2 x} \right)^2 + \cdots + M \left(\frac{\partial u}{\partial x} \right)^3 + \cdots \right], \qquad (\text{I}.14)$$

which after Fourier transformation gives

$$\begin{aligned}
\mathcal{V}[u] = & \int \frac{dk}{2\pi} \left[\frac{K}{2} k^2 + \frac{L}{2} k^4 + \cdots \right] |u(k)|^2 \\
& - iM \int \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} k_1 k_2 (k_1 + k_2) u(k_1) u(k_2) u(-k_1 - k_2) + \cdots.
\end{aligned} \qquad (\text{I}.15)$$

As $k \to 0$, higher order gradient terms (such as L) become unimportant. Also, for small deformations we may neglect terms beyond second order in u (such as M). Adding the kinetic energy, we get a simple one dimensional field theory, with a Hamiltonian

$$\mathcal{H} = \frac{\rho}{2} \int dx \left[\left(\frac{\partial u}{\partial t} \right)^2 + v^2 \left(\frac{\partial u}{\partial x} \right)^2 \right].$$

This is a one–dimensional elastic (string) theory with material dependent constants ρ and $v = \sqrt{K/\rho}$. While the phenomenological approach cannot tell us the value of these parameters, it does show that the low energy excitations satisfy the dispersion relation $\omega = v|k|$.

We can now generalize the elastic theory of the string to arbitrary dimensions d: The discrete particle deformations $\vec{u}_n$ are coarse grained into a continuous deformation field $\vec{u}(\vec{x})$. For an *isotropic* material the potential energy $\mathcal{V}[\vec{u}]$, must be invariant under both rotations and translations $u_\alpha(\vec{x}) \mapsto R_{\alpha\beta}u_\beta(\vec{x}) + c_\alpha$, where $R_{\alpha\beta}$ is a rotation matrix. A useful local quantity is the symmetric *strain field*,

$$u_{\alpha\beta}(\vec{x}) = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right), \tag{I.16}$$

in terms of which the most general quadratic deformation Hamiltonian is

$$\mathcal{H} = \sum_{\alpha,\beta} \int d^d\vec{x} \left[\frac{\rho}{2}\frac{\partial u_\alpha}{\partial t}\frac{\partial u_\alpha}{\partial t} + \frac{2\mu}{2}u_{\alpha\beta}u_{\alpha\beta} + \frac{\lambda}{2}u_{\alpha\alpha}u_{\beta\beta}\right]. \tag{I.17}$$

The elastic constants μ and λ are known as *Lame coefficients*. Summing over the repeated indices ensures that the result is rotationally invariant. This rotational invariance is more transparent in the Fourier basis, $\vec{u}(\vec{k}) = \int d^d\vec{x}e^{i\vec{k}.\vec{x}}\vec{u}(\vec{x})$, since the Hamiltonian

$$\mathcal{H} = \int \frac{d^d\mathbf{k}}{(2\pi)^d}\left[\frac{\rho}{2}|\dot{\vec{u}}(\vec{k})|^2 + \frac{\mu}{2}k^2|\vec{u}(\vec{k})|^2 + \frac{\mu+\lambda}{2}\left(\vec{k}.\vec{u}(\vec{k})\right)^2\right], \tag{I.18}$$

manifestly includes only rotationally invariant quantities $\vec{k} \cdot \vec{k}$, $\vec{u} \cdot \vec{u}$, and $\vec{k} \cdot \vec{u}$. We can further decompose the Hamiltonian into two types of sound modes: *longitudinal modes* where $\vec{k} \parallel \vec{u}$, with $v_\ell = \sqrt{(2\mu+\lambda)/\rho}$, and *transverse modes* with $\vec{k} \perp \vec{u}$, where $v_t = \sqrt{\mu/\rho}$. The internal energy is then given by

$$E(t) = L^d \int \frac{d^d\mathbf{k}}{(2\pi)^d}\left[\frac{\hbar v_\ell k}{\exp(\hbar v_\ell k/k_BT) - 1} + \frac{(d-1)\hbar v_t k}{\exp(\hbar v_t k/k_BT) - 1}\right] \approx \mathcal{A}(v_\ell, v_t)L^d(k_BT)^{d+1}. \tag{I.19}$$

The specific heat vanishes as $C \propto T^d$, as $T \to 0$.

Note:

(1) All material dependent parameters end up in the coefficient $\mathcal{A}$, while the scaling with T is *universal*.

(2) The universal exponent originates from the (hydrodynamic) modes with $\vec{k} \to 0$. The high frequency (short wavelength) modes come into play only at high temperatures.

(3) The scaling exponent depends on dimensionality and the range of interactions. (Long–range Coulomb interactions lead to a different result.)

(4) Experimental observation of a power law alerts us to the physics. For example, in superfluid helium, the observation of $C \propto T^3$ (as opposed to $C \propto T^{3/2}$ expected for an ideal Bose gas), immediately implies phonon–like excitations as noted by Landau.

$\star$ There are many other well known examples demonstrating the universality and importance of power laws. For example, consider a cloud of tracers moving in some unspecified medium. The scaling of some characteristic dimension x with time t can alert us to the possible dynamics that governs the motion of the particles. Three simple possibilities are:

(1) *Diffusion,* in which case $x \propto \sqrt{Dt}$.

(2) *Dissipate transport,* where $x \propto vt$.

(3) *Free forced motion,* where $x \propto gt^2/2$, as in a gravitational field.

The Navier–Stokes equation for fluid flow is yet another example. We can use these examples to construct general guidelines for setting up and analysing phenomenological field theories. Some of steps in the procedure are:

(1) **Input** for construction of the coarse grained Hamiltonian comes from symmetry, range of interactions, and dimensionality.

(2) Unlike the above example, in general nonlinearities cannot be ignored in the resulting effective field theory. We shall learn how to treat such nonlinearities by the methods of perturbation theory and the renormalization group.

(3) **Output** of the analysis is expressed in terms of universal exponents, and other functional dependances that can be directly compared with experiments.