

# Chapter 2

## Quantum statistical mechanics from classical

### 2.1 A lightning review of quantum mechanics

A quantum-mechanical system, many-body or single-body, is defined by two basic objects: a *Hilbert space*, and a *Hamiltonian* acting on it. A Hilbert space is a vector space that has an inner product: a way of taking two vectors and producing a scalar in  $\mathbb{C}$ . The inner product is a natural generalization of a dot product. Each vector in the Hilbert space describes a possible physical state of the system. It is customary in physics to label each state as  $|v\rangle$ , and the inner product of two vectors  $|v\rangle$  and  $|w\rangle$  as  $\langle v|w\rangle$ . This notation emphasizes the fact that the state in a quantum mechanical system is indeed an element of a vector spaces, so that it makes sense to *add* different states together. This phenomenon, called *superposition*, is what is fundamentally weird about quantum behavior. One consequence, described in depth in this chapter, is that a quantum many-body system has physical behavior precisely related to a classical many body system in one higher dimension.

In a Hilbert space, the inner product has the properties that

- Complex conjugation under exchange:

$$\langle v|w\rangle = \langle w|v\rangle^*$$

- Positive definite:

$$\langle v|v\rangle \geq 0$$

with the equality holding only when  $|v\rangle = 0$ .

- Behavior under superposition:

$$\langle w|av_1 + bv_2\rangle = a\langle w|v_1\rangle + b\langle w|v_2\rangle .$$

Note that these properties imply

$$\langle aw_1 + bw_2 | v \rangle = a^* \langle w_1 | v \rangle + b^* \langle w_2 | v \rangle .$$

It is important to note that given a vector space, the inner product is not unique –it must be specified.

Once a Hilbert space  $V$  specified, than a *basis* is a set of states  $\{|j\rangle\}$  and any element of  $V$  can be written as a unique sum over basis states  $|v\rangle = \sum_j \alpha_j |j\rangle$ . The number of basis states is called the *dimension* of  $V$ . An *orthonormal basis* is one where basis states obey  $\langle i | j \rangle = \delta_{ij}$ . In an orthonormal basis,  $\alpha_j = \langle j | v \rangle$ . Another orthonormal basis  $\{|\tilde{j}\rangle\}$  can be obtained by multiplying the basis elements by any unitary matrix  $U$  of size  $V \times V$ :  $|\tilde{j}\rangle = \sum_j U_{ij} |j\rangle$ . It is easy to check that this preserves all the appropriate properties of the Hilbert space.

A Hamiltonian is a linear self-adjoint operator  $H$  which takes  $V$  to itself, i.e. maps each element of  $V$  to some other element of  $v$ . The usual physicist notation for this is that  $H$  takes  $|v\rangle$  to  $H|v\rangle = |Hv\rangle$ . *Linearity* is an essential property of quantum mechanics, and it means that  $H(|v_1\rangle + |v_2\rangle) = H|v_1\rangle + H|v_2\rangle$ . The linearity means that in a particular basis, the Hamiltonian is represented as a matrix whose elements are given by

$$H_{ji} = \langle i | H | j \rangle$$

so that the action of  $H$  on a state in this basis is a matrix whose entries are  $H_{ij}$ . Namely, the  $i$ th component of the vector  $|Hv\rangle$  in this basis is given by

$$\langle i | Hv \rangle = \langle i | H | v \rangle = \sum_j H_{ij} \langle j | v \rangle .$$

Such relations are often easy to find by “inserting a complete set of states”, or a ”partition of unity”, i.e. exploiting the fact that in an orthonormal basis

$$1 = \sum_j |j\rangle \langle j| . \tag{2.1}$$

Both sides in this relation should be interpreted as operators taking  $V$  to  $V$ , so the left-hand side is the identity operator, while each term on the right hand side means taking the inner product with the basis state  $\langle j|$  and mapping it to  $|j\rangle$ .

The Hamiltonian gives the *time evolution* of a state. If the system is in a state  $|v_0\rangle$  at some time  $t_0$ , then at a later time  $t_1$ , the system is therefore in the state

$$e^{-iH(t_1-t_0)/\hbar} |v_0\rangle .$$

The exponential of any operator is always understood as a power series. Put another way, the time dependence of any state is given by the first-order differential equation

$$i\hbar \frac{\partial}{\partial t} |v(t)\rangle = H |v(t)\rangle .$$

The eigenstates and eigenvalues of the Hamiltonian therefore play a very special role. For each eigenvalue  $E$  the corresponding eigenstate  $|E\rangle$  evolves in time only with a phase:

$$|E(t_1)\rangle = e^{-iH(t_1-t_0)/\hbar}|E_0\rangle .$$

These eigenvalues are the *energy levels* of the system, and the eigenstates of  $H$  are called *stationary states*).

The partition function in a quantum system is therefore defined in a quite analogous manner to the classical system:

$$Z = \sum_j e^{-\beta E_j} .$$

In fact, for a system in finite volume, this is a better-defined object than the classical partition function, since the quantum energies take on a set of countable values. Put more technically, it puts a natural measure on phase space. The partition function of a quantum system can be rewritten in a very provocative fashion. Letting the  $|E_j\rangle$  be the orthonormalized stationary states gives

$$\begin{aligned} Z &= \sum_j \langle E_j | e^{-\beta E_j} | E_j \rangle = \sum_j \langle E_j | e^{-\beta H} | E_j \rangle \\ &= \text{tr } e^{-\beta H} \end{aligned} \tag{2.2}$$

The latter form has the distinct advantage of being independent of basis, so one does *not* need to compute the energy eigenvalues explicitly in order to compute or approximate  $Z$ .

## 2.2 The quantum/classical correspondence

At zero temperature,  $\beta \rightarrow \infty$ , so the partition function ((2.2) of a quantum system is therefore dominated by the *ground state*, the state (or states) with the lowest energy  $E_0$ :

$$Z \approx e^{-\beta E_0}$$

Thus the ground state energy of the quantum system is akin to the minimum of the free energy in the classical case. More importantly, the partition function of the quantum system is dominated by the ground *state*  $|\Psi_0\rangle$  of the quantum system, just like the classical partition function is dominated by the equilibrium state, the set of configurations at the energy where the free energy is a minimum.

The correspondence thus extends to expectation values as well. Namely, when  $\mathcal{O}$  is some operator in the quantum system, its expectation value in a given state  $|\Psi\rangle$  is by definition  $\langle \Psi | \mathcal{O} | \Psi \rangle$ . Thus at zero temperature, the expectation value is simply  $\langle \Psi_0 | \mathcal{O} | \Psi_0 \rangle$ . Writing the ground state in an orthonormal basis as  $|\Psi_0\rangle = \sum_j \alpha_j |j\rangle$  means that when  $\mathcal{O}$  is diagonal in this basis, its zero-temperature expectation value is  $\sum_j |\alpha_j|^2 \mathcal{O}_j$ .

Likewise, when the partition sum in a classical model is dominated by the equilibrium configurations, expectation values become of the form  $\sum_j \mathcal{O}_j$ , where  $j$  labels the configurations at the free energy minimum.

One way of gaining intuition into the correspondence between classical many-body systems at non-zero temperature and quantum systems at zero temperature is think about the role of fluctuations in both case. Both kinds of systems are necessarily described by probabilities. In the classical case, this is because thermal equilibrium is treated by imagining the system as being coupled to a large bath at constant temperature, so that the coupling causes fluctuations in the original system. The temperature plays an essential role in weighting the different configurations appropriately. In the quantum case, uncertainty is fundamental to the whole enterprise. Thus the behavior of a zero-temperature many-body quantum is as rich as as a classical system at non-zero temperature.

This correspondence between classical and quantum is even deeper, and can be made more precise. The similarity of  $e^{-\beta H}$  with the quantum-mechanical time-evolution operator  $e^{-iHt/\hbar}$  is entirely not coincidental. As noted in the chapter 1, the best way to think intuitively of a transfer matrix is as a discrete “evolution” operator across one dimension of space, acting on one slice at a time. The transfer matrix acts on a vector space of states in one dimension smaller, the space of possible boundary conditions. For  $L$  slices the partition function is then found by taking  $T^{L-1}$  to act the particular choice of boundary conditions, or  $Z = \text{tr } T^L$  if the boundary conditions are periodic. Thus if one takes  $\Delta\tau = \beta/L$ , a sort of Hamiltonian can be defined via

$$\mathcal{H} \equiv \frac{1}{\Delta\tau} \ln(T) ,$$

so that e.g.

$$Z = \text{tr} (e^{-\mathcal{H}\Delta\tau})^{\beta/\Delta\tau} = \text{tr} e^{-\beta\mathcal{H}}$$

for periodic boundary conditions. This is thus formally equivalent to the partition function of a quantum system in *one dimension less*. The Hilbert space is the vector space of boundary conditions; for example in a spin model the basis elements are the different configurations of spins at the boundary.

Conversely, given a quantum Hamiltonian, one can think of the quantum partition function  $Z = \text{tr} e^{-\beta H}$  as being time evolution over a continuous *imaginary time*. A sort of transfer matrix then evolves the system for an infinitesimal time, i.e.  $\mathcal{T} = e^{-H\delta\tau}$ . To get the partition function, this transfer matrix evolves a distance  $\beta$  in this imaginary time, with the trace corresponding to periodic boundary conditions. Thus this corresponds to a classical system in one higher dimension, with this extra dimension having size  $\beta\hbar$  and periodic boundary conditions.

Unfortunately, the quantum/classical correspondence is not as simple as this. The catch is that  $\mathcal{H}$  is typically impossible to compute. Even if it were, it is a highly non-local object even for  $T$  is local, since taking  $\ln T$  results in a power series. This would-be

Hamiltonian  $\mathcal{H}$  would thus describe strong interactions at long distances and does not therefore does not correspond to the Hamiltonian of a physical system.

However, in many situations of interest, a miracle occurs. A *quantum many-body system in  $d$  spatial dimensions* has the *same* physical properties as a classical many-body system in  $d + 1$  dimensions. In the limit of an infinite number of degrees of freedom, the correspondence is exact: appropriately-defined physical quantities are the same in the classical and quantum theories. The reasons for the miracle take a while to explain, and so will emerge in the following chapters. The one-sentence explanation is that at and near a critical point the physics at long-distance becomes independent of much of the short-distance behavior, and so the same field theory describes both classical and quantum models.

A difference in language is worth noting. Particle physicists and others who study quantum field theory typically refer to the *space-time* dimensions of a system; e.g. the universe we know is four-dimensional, or ten-dimensional in superstring theory, or 11-dimensional in  $M$  theory. Condensed matter physicists, whether they are studying quantum or classical physics, typically describe a system by the number of *spatial* dimensions, so that the universe we know is three-dimensional. Often to avoid confusion in these situations, systems are referred to as being in  $d + 1$  dimensions. This is a nice convention, although be warned that there is also some ambiguity here, since often this is meant to imply also that the theory is Lorentz invariant, a situation that usually (but not always) occurs in particle physics, and that frequently (but far from always) occurs in condensed-matter physics. Moreover, quantum effects are negligible in many interesting condensed matter systems, so the spatial dimension of the system is precisely the dimension of the field theory describing the system.

The first step in understanding this correspondence is to find the quantum Hamiltonian associated with a given classical system. A quantum Hamiltonian can be used to evolve a system for an infinitesimal imaginary time, so the system after this infinitesimal evolution is very close to the original:

$$e^{-H\delta\tau} \sim 1 - H\delta\tau .$$

Thus a quantum Hamiltonian corresponding to a given classical system can be found if the couplings of the classical system can be tuned so that the transfer matrix is very close to the identity, i.e.  $H$  is defined via

$$T \sim 1 - H\delta\tau .$$

Heuristically, this can be thought of as tuning the couplings of the classical model to make the slices “close” together. The precise definition of  $\delta\tau$  here is not important because the overall scale of a quantum Hamiltonian simply amounts to the overall energy scale; all that is important is that  $\delta\tau$  is small.

The simplest example is the one-dimensional classical Ising model discussed in depth

in the previous chapter. For a classical energy including a magnetic field

$$E = -J \sum_i \sigma_i \sigma_{i+1} - h \sum_i \sigma_i ,$$

the transfer matrix is

$$T = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix} = e^{\beta J} \cosh(\beta h) \begin{pmatrix} 1 + \tanh(\beta h) & e^{-2\beta J} \\ e^{-2\beta J} & 1 - \tanh(\beta h) \end{pmatrix} \quad (2.3)$$

This transfer matrix acts on a two-dimensional vector space with basis elements corresponding to the spin up and spin down states at the boundary. Taking  $\beta h \rightarrow 0$ ,  $\beta J \rightarrow \infty$  while keeping the combination

$$\alpha = e^{2\beta J} \tanh(\beta h) \quad (2.4)$$

finite gives

$$T \approx \text{const.} \times (I + e^{-2\beta J} (\sigma^x + \alpha \sigma^z)) ,$$

where  $I$  is the identity matrix and  $\sigma^x$  and  $\sigma^z$  the Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The overall constant in front can be ignored since it multiplies the partition function by an overall constant, and so merely shifts the energy uniformly.

The associated quantum Hamiltonian is now easy to extract by identifying  $\delta\tau = e^{-2\beta J}$ , yielding

$$H = -\sigma^x - \alpha \sigma^z \quad (2.5)$$

These matrices are two-dimensional, so the Hilbert space for the associated quantum system is two dimensional. Thus this is the simplest non-trivial quantum system, often called a fixed quantum spin-1/2 particle, or more simply, a “two-state” quantum system. The two terms are typically known respectively as a “transverse magnetic field” and just plain “magnetic field”. The off-diagonal transverse field arises in the quantum Hamiltonian because in the classical model the spins of course can vary as one moves from slice to slice.

In this simple case, it is easy to check that  $[T, H] = 0$ , and so the transfer matrix and the Hamiltonian have the same eigenvectors. In this special case, the physics of the quantum classical models is obviously the same. Although having a transfer matrix commute with the Hamiltonian is not typical behavior, such behavior occurs frequently in certain models in 1+1 dimensions. Such models are called *integrable*, and as a consequence some quantities can be computed exactly by using techniques such as the Bethe ansatz.

Local quantum Hamiltonians associated with a given classical model are typically not difficult to find, as long as the couplings in the classical model can be tuned to make

the transfer matrix close to the identity. This usually can be done, although some tricks often need to be applied. For example, in the 0 + 1-dimensional antiferromagnetic Ising model with  $J < 0$ , one can no longer take  $e^{-2\beta J} \rightarrow 0$ , since  $\beta$  is by definition positive. For  $h = 0$ , a Hamiltonian can be found by redefining states by flipping every other spin. For  $h \neq 0$ , that trick results in a system no longer translation invariant (the field is staggered), so the Hamiltonian can only be found by taking the limit of  $T^2$ .

## 2.3 The quantum Ising Hamiltonian

The quantum-classical correspondence is nicely illustrated by finding the quantum Hamiltonian associated with the Ising model.

It is simplest to start with the 1+1-dimensional case of the Ising model on a square lattice. The transfer matrix acts on a one-dimensional slice of spins, the vector space spanned by the set of all spins along the slice. Thus the resulting quantum Hamiltonian will act on a many-body system of spins in a row, so that this and similar one-dimensional quantum systems are typically referred to as “chains”.

The building blocks of the transfer matrix each arise from a single link. For a transfer matrix acting in the  $x$  direction, the horizontal and vertical links give rise to very different building blocks. To find a limit where the transfer matrix is close to the identity, it is necessary to take different couplings in the  $x$  and  $y$  direction. For a link in the horizontal direction, the situation is akin to the one dimensional example, which consists entirely of horizontal links. For each row, there is a building block

$$W_i = \begin{pmatrix} e^{\beta J_x} & e^{-\beta J_x} \\ e^{-\beta J_x} & e^{\beta J_x} \end{pmatrix} = e^{\beta J_x} (I + e^{-2\beta J_x} \sigma_i^x). \quad (2.6)$$

The fact that for a link in the vertical direction, the transfer matrix is diagonal, measuring whether or not the two spins are the same:

$$\begin{aligned} V_{i,i+1} = e^{\beta J_y \sigma_i^z \sigma_{i+1}^z} &= \cosh(\beta J_y) + \sigma_i^z \sigma_{i+1}^z \sinh(\beta J_y) \\ &= \cosh(\beta J_y) (1 + \tanh(\beta J_y) \sigma_i^z \sigma_{i+1}^z) \end{aligned} \quad (2.7)$$

With free boundary conditions in the  $y$  direction, the transfer matrix for  $N$  sites in each column is

$$T = \left( \prod_{i=1}^{N-1} V_{i,i+1} \right) \left( \prod_{j=1}^N W_j \right)$$

For periodic boundary conditions in the  $y$  direction, the first product goes to  $N$  instead, with the indices interpreted mod  $N$ . The different  $V$  commute among themselves, as do the  $W$ . However  $V_{i,i+1}$  does not commute with  $W_i$  or  $W_{i+1}$ , making the  $T$  a very non-trivial matrix.

For  $M$  sites and periodic boundary conditions in the  $x$  direction, so that there are  $NM$  sites in all, the partition function is

$$Z = \text{tr}(T)^M .$$

The partition function for other boundary conditions in the  $x$  direction can be found in the same fashion as described in chapter 1, by having  $T$  act on a particular vector, so that

$$Z = v^T T^{M-1} w .$$

In this 1+1 dimensional case, this vector space is  $2^N$  dimensional. The vector corresponding to free boundary conditions has a 1 in each of the  $2^N$  components, while for fixed boundary conditions, the vector is zero in all components save one, the basis element corresponding to the particular fixed configuration (e.g. all spins up).

Finding a limit where  $T$  is near the identity is very similar to the 0+1-dimensional case. The appropriate limit is

$$e^{-2\beta J_x} \rightarrow 0, \quad \tanh(\beta J_y) \rightarrow 0$$

with

$$\lambda \equiv e^{2\beta J_x} \tanh(\beta J_y) \tag{2.8}$$

remaining finite. Notice this means that  $J_x \rightarrow \infty$ , while  $J_y \rightarrow 0$ . Therefore the Hamiltonian for the *quantum Ising chain* with free boundary conditions is

$$H = -\lambda \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^N \sigma_i^x . \tag{2.9}$$

The quantum Hamiltonian of course does not depend on the boundary conditions in the  $x$  direction, but does depend on the choice in  $y$ . Thus for periodic boundary conditions for the latter, the first sum goes to  $N$  instead.

Generalizing this to higher-dimensional cubic lattice is now obvious. One direction, say the  $x$  one, is singled out as imaginary time, and then  $J_x$  is sent to  $\infty$ , so that the sites in this direction become effectively close to each other. The sites with a fixed value of  $x$  form a single slice. The couplings in the directions along the slice (i.e. the directions other than  $x$ ) can be chosen to be the same, and then a finite  $\lambda$  is defined as in (2.8). The quantum Ising Hamiltonian in then any dimension for  $N$  sites on each slice is therefore

$$H = -\lambda \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \sum_{i=1}^N \sigma_i^x . \tag{2.10}$$

Sometimes this quantum Ising model is referred to as the “Ising model in a transverse field”, because of the presence of the  $\sigma^x$  terms. While the nomenclature is fine, it is important to remember that this model describes the classical model with no field at



all. As with the 0+1-dimensional case, the transverse field terms arise because the spins change slice-to-slice.

Analyzing such many-body quantum Hamiltonians is a central part of statistical mechanics. The remainder of this book will discuss the Ising Hamiltonian and others in great depth. In particular, in chapter 4, I will explain how to exactly compute the ground-state energy of the quantum Ising chain.