3

Path integrals and statistical mechanics

The Feynman path integral formulation of quantum mechanics reveals deep connections with statistical mechanics. This chapter is concerned with this relationship for the simple case of a non-relativistic particle in a potential. Starting with a partition function representing a path integral on an imaginary time lattice, we will show how a transfer matrix formalism reduces the problem to the diagonalization of an operator in the usual quantum mechanical Hilbert space of square integrable functions (Creutz, 1977). In the continuum limit of the time lattice, we obtain the canonical Hamiltonian. Except for our use of imaginary time, this treatment is identical to that in Feynman's early work (Feynman, 1948).

We begin with the Lagrangian for a free particle of mass m moving in potential $V(x)$

$$L(x, \dot{x}) = K(\dot{x}) + V(x), \tag{3.1}$$

$$K(\dot{x}) = \tfrac{1}{2}m\dot{x}^2, \tag{3.2}$$

where $\dot{x}$ is the time derivative of the coordinate x. Velocity-dependent potentials are beyond the scope of this book. Note the unconventional relative positive sign between the two terms in eq. (3.1). This is because we formulate the path integral directly in imaginary time. This improves mathematical convergence, yet leaves us with the usual Hamiltonian for diagonalization.

For any trajectory we have an action

$$S = \int \mathrm{d}t\, L(\dot{x}(t), x(t)), \tag{3.3}$$

which appears in the path integral

$$Z = \int [\mathrm{d}x(t)]\, \mathrm{e}^{-S}. \tag{3.4}$$

Here the integral is over all trajectories $x(t)$. As it stands, eq. (3.4) is rather poorly defined. To characterize the possible trajectories we introduce a cutoff in the form of a time lattice. Putting our system into a time box of total length τ, we divide this interval into

$$N = \tau/a, \tag{3.5}$$

discrete time slices, where a is the timelike lattice spacing. Associated with the i'th such slice is a coordinate x_i. This construction is sketched in figure 3.1. Replacing the time derivative of x with a nearest-neighbor difference, we reduce the action to a sum

$$S = a\sum_i\left[\tfrac{1}{2}m\left(\frac{x_{i+1}-x_i}{a}\right)^2 + V(x_i)\right]. \tag{3.6}$$

The integral in eq. (3.4) is now defined as an integral over all the coordinates

$$Z = \int\left(\prod_i \mathrm{d}x_i\right)\mathrm{e}^{-S}. \tag{3.7}$$

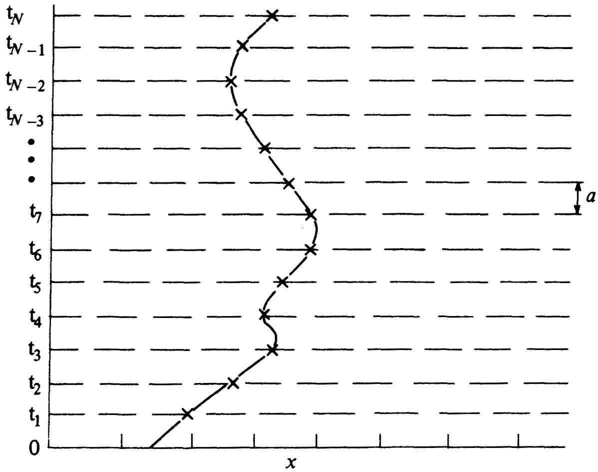

Fig. 3.1. Dividing time into a lattice. (From Creutz and Freedman, 1981.)

Eq. (3.7) is precisely in the form of a partition function for a statistical system. We have a one-dimensional chain of coordinates x_i. The action represents the inverse temperature times the Hamiltonian of the thermal analog. We will now show that evaluation of this partition function is equivalent to diagonalizing a quantum mechanical Hamiltonian obtained from this action with canonical methods. This is done via the transfer matrix.

The key to the transfer-matrix analysis is to note that the local nature of the action in eq. (3.6) permits us to write the partition function in the form of a matrix product

$$Z = \int\prod_i \mathrm{d}x_i\, T_{x_{i+1},\,x_i}, \tag{3.8}$$

where the transfer-matrix elements are

$$T_{x',x} = \exp\left[-\frac{m}{2a}(x'-x)^2 - \frac{a}{2}(V(x')+V(x))\right]. \tag{3.9}$$

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This operator acts in the Hilbert space of square integrable functions, where the inner product is the standard

$$\langle \psi' | \psi \rangle = \int dx\, \psi'^*(x)\, \psi(x). \tag{3.10}$$

We introduce the non-normalizable basis states $\{|x\rangle\}$ such that

$$|\psi\rangle = \int dx\, \psi(x)\, |x\rangle, \tag{3.11}$$

$$\langle x' | x \rangle = \delta(x'-x), \tag{3.12}$$

$$1 = \int dx\, |x\rangle \langle x|. \tag{3.13}$$

The canonically conjugate operators $\hat{p}$ and $\hat{x}$ satisfy

$$\hat{x}\,|x\rangle = x\,|x\rangle, \tag{3.14}$$

$$[\hat{p}, \hat{x}] = -\mathrm{i}, \tag{3.15}$$

$$e^{-\mathrm{i}\hat{p}\Delta}|x\rangle = |x+\Delta\rangle. \tag{3.16}$$

In this Hilbert space the operator T is defined via its matrix elements

$$\langle x' | T | x \rangle = T_{x',x}, \tag{3.17}$$

where $T_{x',x}$ is given in eq. (3.8). With periodic boundary conditions for our lattice of N sites, the path integral is compactly expressed

$$Z = \mathrm{Tr}\,(T^N). \tag{3.18}$$

The operator T is easily written in terms of the conjugate variables $\hat{p}$ and $\hat{x}$

$$T = \int d\Delta\, e^{-aV(\hat{x})/2}\, e^{-\Delta^2 m/(2a) - \mathrm{i}\hat{p}\Delta}\, e^{-aV(\hat{x})/2}. \tag{3.19}$$

To prove this equation, simply check that the right hand side has the matrix elements of eq. (3.9). The integral over Δ is Gaussian and gives

$$T = (2\pi a/m)^{\frac{1}{2}}\, e^{-\frac{1}{2}aV(\hat{x})}\, e^{-\frac{1}{2}a\hat{p}^2/m}\, e^{-\frac{1}{2}aV(\hat{x})}. \tag{3.20}$$

Connection with the usual quantum mechanical Hamiltonian appears in the small lattice spacing limit. When a is small, the exponents in eq. (3.20) combine to give

$$T = (2\pi a/m)^{\frac{1}{2}}\, e^{-aH+O(a^3)}, \tag{3.21}$$

where

$$H = \hat{p}^2/(2m) + V(\hat{x}). \tag{3.22}$$

This is just the canonical Hamiltonian corresponding to the Lagrangian in eq. (3.1).

The procedure for going from a path-integral to a Hilbert-space formulation of quantum mechanics consists of three steps. First define the path integral with a time lattice. Then construct the transfer matrix and the Hilbert space on which it operates. Finally, take the logarithm of the transfer matrix and identify the negative of the coefficient of the linear term in the lattice spacing as the Hamiltonian. Physically, the transfer matrix propagates the system from one time to the next. Such time translations are generated by the Hamiltonian. Denoting the i'th eigenvalue of the transfer matrix by λ_i, eq. (3.18) becomes

$$Z = \sum_i \lambda_i^N. \tag{3.23}$$

As the number of time slices goes to infinity, this expression is dominated by the largest eigenvalue λ_0

$$Z = \lambda_0^N \times [1 + O(\exp[-N \ln(\lambda_0/\lambda_1)])]. \tag{3.24}$$

Thus in statistical mechanics the thermodynamic properties of a system follow from this largest eigenvalue. In ordinary quantum mechanics the corresponding eigenvector is the lowest eigenstate of the Hamiltonian; it is the ground state or, in field theory, the vacuum. Note that in this discussion the connection between imaginary and real time is trivial. Whether the generator of time translations is H or $\mathrm{i}H$, we still have the same operator to diagonalize.

In statistical mechanics one is often interested in correlation functions of the statistical variables. This corresponds to a study of the Green's functions of the corresponding field theory. These are obtained upon insertion of polynomials of the fundamental variables into the path integral. We define the two-point function

$$\langle x_i x_j \rangle = (1/Z) \int \left(\prod_k \mathrm{d}x_k \right) x_i x_j \, \mathrm{e}^{-S}. \tag{3.25}$$

In terms of the transfer matrix, this reduces, for positive $i-j$, to

$$\langle x_i x_i \rangle = (1/Z) \operatorname{Tr}(T^{N-i+j} \hat{x} T^{i-j} \hat{x}). \tag{3.26}$$

Taking the length of our time box to infinity while holding the separation of i and j fixed we obtain

$$\langle x_i x_j \rangle = \langle 0 | \hat{x} (T/\lambda_0)^{i-j} \hat{x} | 0 \rangle, \tag{3.27}$$

where $|0\rangle$ is the ground state, which dominated in eq. (3.24). For a continuum limit, we hold the physical time between i and i fixed

$$t = (i-j)\,a, \tag{3.28}$$

and let a go to zero. We now introduce the time-dependent operator

$$\hat{x}(t) = \mathrm{e}^{Ht} \hat{x} \, \mathrm{e}^{-Ht}, \tag{3.29}$$

which corresponds to the quantum mechanical coordinate in the Heisenberg representation, but rotated to our imaginary time. Defining a time-ordering instruction to include negative time separations in the

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above, we identify

$$\begin{aligned}\langle x_i x_j \rangle &= \langle 0|\mathscr{T}(\hat{x}(t)\,\hat{x}(0))|0\rangle \\ &= \theta(t)\,\langle 0\,|\,\hat{x}(t)\,\hat{x}(0)\,|\,0\rangle + \theta(-t)\,\langle 0\,|\,\hat{x}(0)\,\hat{x}(t)\,|\,0\rangle, \end{aligned} \tag{3.30}$$

where

$$\theta(t) = \begin{Bmatrix} 1, & t \geqslant 0 \\ 0, & t < 0. \end{Bmatrix} \tag{3.31}$$

This is a general result; the correlation functions of the statistical analog correspond directly with the time-ordered products of the corresponding quantum fields. It is precisely this point which allows the particle physicist to borrow technology from statistical mechanics.

In this chapter we have seen that statistical mechanics and quantum mechanics have deep mathematical connections. In general, a d-space-time dimensional quantum field theory is equivalent to a d-Euclidian dimensional classical statistical system.

Quantum statistical mechanics can also be related to quantum field theory. If we combine eqs (3.18) and (3.21) we obtain

$$Z = (2\pi a/m)^{N/2}\,\mathrm{Tr}(\mathrm{e}^{-aNH}). \tag{3.32}$$

If we now identify

$$T = (aN)^{-1}, \tag{3.33}$$

and do not go to the large time limit, we see that a path integral in a periodic temporal box is itself a partition function at a temperature corresponding to the inverse of this periodic time. Thus the path integral formulation also enables us to study the quantum statistical mechanics of the original $(d-1)$-space dimensional theory. We will return to this point when we discuss gauge theories at finite physical temperatures and the resulting deconfining phase transitions.

Problems

1. Consider the harmonic oscillator with $V(x) = \frac{1}{2}kx^2$. Diagonalize the operator T of eq. (3.20). (Hint: find an operator of form $\frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$ which commutes with T and can thus be simultaneously diagonalized.) (Creutz and Freedman, 1981.)

2. In the harmonic oscillator example, find the 'propagator' $\langle x_i x_j \rangle$.

3. Show that $a^{-2}\langle (x_{i+1} - x_i)^2 \rangle$ diverges as a goes to zero. Show that the split point product $a^{-2}\langle (x_{i+1} - x_i)(x_i - x_{i-1}) \rangle$ approaches $-\langle 0\,|\,p^2\,|\,0\rangle$ in the continuum limit. Where does the minus sign come from?

4. Calculate the fluctuations in the propagator:

$$D^2(i, j) = \langle (x_i x_j)^2 \rangle - \langle x_i x_j \rangle^2.$$

Show that the fluctuations in the split point product of problem 2 diverge as a goes to zero. Derive the virial theorem for the continuum theory:

$$\langle 0 | \hat{p}^2 | 0 \rangle = \langle 0 | \hat{x} V'(\hat{x}) | 0 \rangle.$$

This gives the average momentum squared without large fluctuations.

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