Chapter 6

Functional Methods in Quantum Mechanics

So far we have focused on studies of classical statistical mechanics. However, a very important analogy, which we will develop and exploit below, exists between the quantum mechanics of a d-dimensional system and the classical statistical mechanics of a $d+1$-dimensional system.

6.1 Feynman Path Integral

The original suggestion of an alternative representation of quantum mechanical amplitudes in terms of path integrals stems from the work of Dirac (1933) and was developed by Feynman in the 1940's. Although this method was, at first, received with some suspicion by the community, it became clear in the 1970's that it is the most flexible tool for developing ideas in field theory of high energy and condensed matter physics.

The path integral involves a functional representation of the quantum mechanical time evolution operator. To derive it we start with the time dependent Schrödinger equation

$$\boxed{i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle}$$

Formally, the latter can be integrated to give an expression for the time evolution operator

$$\boxed{|\Psi(t')\rangle = \hat{U}(t',t)|\Psi(t)\rangle, \qquad \hat{U}(t',t) = \exp\left[-\frac{i}{\hbar}\hat{H}(t'-t)\right]}$$

In the real space representation we can write

$$\Psi(x',t') = \langle x'|\Psi(t')\rangle = \langle x'|\hat{U}(t',t)\Psi(t)\rangle = \int dx U(x',t';x,t)\Psi(x,t),$$

where

$$U(x',t';x,t) = \langle x'|\exp\left[-\frac{i}{\hbar}\hat{H}(t'-t)\right]|x\rangle,$$

defines the (x', x) component of the time evolution operator.

To obtain an expression for $U(x', t'; x, t)$ in the form of an integral over classical paths it is convenient to discretise the time evolution into a sequence of small time steps

$$\hat{U}(t', t) = \hat{U}(t', t_{N-1})\hat{U}(t_{N-1}, t_{N-2}) \cdots \hat{U}(t_1, t),$$

where $t_k = t + k\ \Delta t$ such that $t' - t = N\ \Delta t$ ($t_0 = t$, $t_N = t'$). Eventually we will take the limit $N \to \infty$ and $\Delta t \to 0$. In the real space representation we have

$$\begin{aligned} U(x', t'; x, t) = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \langle x'|\hat{U}(t', t_{N-1})|x_{N-1}\rangle \\ \times \langle x_{N-1}|\hat{U}(t_{N-1}, t_{N-2})|x_{N-2}\rangle\langle x_{N-2}| \cdots \hat{U}(t_1, t)|x\rangle. \end{aligned} \tag{6.1}$$

Taking the time steps to be infinitesimal, for a single term we obtain[1]

$$\begin{aligned} \langle x_{k+1}|\hat{U}(t_{k+1}, t_k)|x_k\rangle &\equiv \langle x_{k+1}|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_k\rangle = \int \frac{dp_k}{2\pi\hbar}\langle x_{k+1}|p_k\rangle\langle p_k|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_k\rangle \\ &= \int \frac{dp_k}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\left(p_k\dot{x}_k - H(p_k, x_k)\right)\Delta t\right] + O(\Delta t)^2. \end{aligned}$$

Inserting this expression into Eq. (6.1) we obtain (see fig. 6.1)

$$\begin{aligned} U(x', t'; x, t) &= \int \frac{dp_{N-1}}{2\pi\hbar} \cdots \int \frac{dp_0}{2\pi\hbar} \int dx_{N-1} \cdots \int dx_1 \\ &\qquad \times \exp\left[\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(p_k\dot{x}_k - H(p_k, x_k)\right)\Delta t\right] \\ &\overset{N\to\infty, \Delta t\to 0}{\to} \int Dp(t'') \int_{x(t)=x}^{x(t')=x'} Dx(t'') \exp\left[\frac{i}{\hbar}\int_t^{t'} dt''\left(p\dot{x} - H(p, x)\right)\right], \end{aligned} \tag{6.2}$$

where the factors of $2\pi\hbar$ are absorbed into the definition of the functional integral. For Hamiltonians quadratic in p the integral is Gaussian and can be performed straightforwardly:

$$p\dot{x} - \frac{p^2}{2m} = -\frac{1}{2m}\left(p - m\dot{x}\right)^2 + \frac{m}{2}\dot{x}^2.$$

As a result we obtain

$$\boxed{U(x', t'; x, t) = \int Dx(t'')Dp(t'') \exp\left[\frac{i}{\hbar}S(p, x)\right] = \int \bar{D}x(t'') \exp\left[\frac{i}{\hbar}S(x)\right]}$$

where

$$\begin{aligned} S(p, x) &= \int_t^{t'} dt''\left[p\dot{x} - H(p, x)\right], \\ S(x) &= \int_t^{t'} dt''\left[\frac{m}{2}\dot{x}^2 - V(x)\right] \end{aligned}$$

[1] By writing the infinitesimal evolution operator in a *normal ordered* form (i.e. by rearranging the expansion such that all momentum operators $\hat{p}$ appear to the left of the position operators $\hat{x}$), show that the difference between $\langle p_k|\exp[-(i/\hbar)\hat{H}\Delta t]|x_k\rangle$ and $\exp[-(i/\hbar)H(p_k, x_k)\Delta t]$ is $O(\Delta t)^2$.

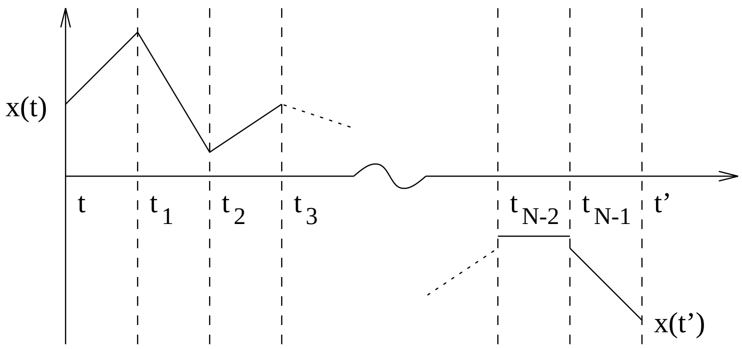

Figure 6.1: A typical trajectory contributing to the path integral.

denote representations of the classical action,[2] and the factors resulting from the dp integrations have been accommodated in the measure

$$\bar{D}x \equiv \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2} dx_1 \cdots dx_{N-1}.$$

For example, it is left as an exercise to show that for a free particle

$$U(x', t'; x, t) = \left(\frac{m}{2\pi i\hbar(t'-t)}\right)^{1/2} \exp\left[\frac{i}{\hbar}\frac{m(x'-x)^2}{2(t'-t)}\right]. \tag{6.3}$$

6.2 Statistical Mechanics

To establish an analogy with statistical mechanics we have to consider propagation in *imaginary* or *Euclidean time* T. Repeating the procedure of the previous section we obtain

$$U(x', t' = -iT; x, t = 0) = \int Dx(\tau) \exp\left[-\frac{1}{\hbar}S(x)\right], \tag{6.4}$$

where

$$S(x) = \int_0^T d\tau \left[\frac{m}{2}\left(\frac{\partial x}{\partial \tau}\right)^2 + V(x(\tau))\right]. \tag{6.5}$$

(Notice that the sign of the potential is *reversed*.) This shows that we have even more freedom in computing the functional integral: The intermediate points t_k can be chosen to

[2]Note that in the semi-classical limit ($\hbar \to 0$), the path integral is dominated by the saddle-point. Minimising the action with respect to variations in δS we find that the saddle-point solution is specified by the classical Hamilton equations of motion

$$\begin{aligned}\delta S(p, x) &= S(p + \delta p, x + \delta x) - S(p, x), \\ &= \int dt'' \left\{\delta p(t'')\left[\dot{x} - \frac{\partial H}{\partial p}\right] + \delta x(t'')\left[-\dot{p} - \frac{\partial H}{\partial x}\right]\right\}.\end{aligned}$$

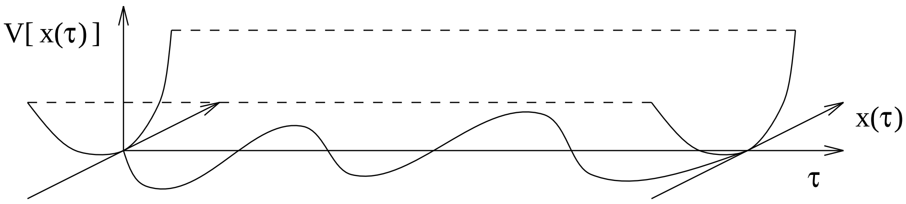

Figure 6.2: A fluctuating string confined to a potential well $V[x]$.

lie on an arbitrary contour in the complex plane. Providing the expression is everywhere convergent ($\mathrm{Im}\Delta t < 0$) time can proceed along some arbitrary complex path.

Let us compare this problem to the classical statistical mechanics of a string. If a string of length T and tension m is allowed to undergo transverse displacements $x(\tau)$, where τ parametrises, *not* time but, the length along the string, the potential energy stored by the string is given by

$$E_{\mathrm{pot}} = m\int_0^T d\tau\left(\left[1+\left(\frac{\partial x}{\partial\tau}\right)^2\right]^{1/2} - 1\right) \approx \frac{m}{2}\int_0^T d\tau\left(\frac{\partial x}{\partial\tau}\right)^2.$$

Straightforward inspection reveals

$$S(x) = E_{\mathrm{pot}}(x),$$

where, in this case, E_{pot} denotes the potential energy of the string with ends fixed at x and x' resting in an additional external potential $V(x)$, "a string in a gutter" (see fig. 6.2). According to the Boltzmann principle, the classical partition function of the string is proportional to

$$\mathcal{Z} \sim \int Dx(\tau)e^{-\beta E_{\mathrm{tot}}} \tag{6.6}$$

where, as usual, $\beta = 1/kT$. Since, in classical statistical mechanics, the contribution from kinetic energy factors out and is independent of x and x' it can, in this case, be omitted.

Comparison of Eq. (6.6) and (6.4) shows the first analogy between classical statistical mechanics and quantum mechanics: *The transition amplitude for a quantum particle for the time (-iT) is equal to the classical partition function for a string of length T computed at the value $\beta = 1/\hbar$.*

The second analogy follows from the fact that the *quantum* partition function for the particle is given by $\mathcal{Z}_{\mathrm{qu}} = \mathrm{Tr}\exp[-\beta H]$ and hence,

$$\mathcal{Z}_{\mathrm{qu}} = \int dx\langle x|e^{-\beta H}|x\rangle = \int dx U(x, t' = -i\beta\hbar; x, t = 0). \tag{6.7}$$

Therefore applying Eq. (6.2) we obtain our second rule: *In quantum statistical mechanics, the inverse temperature plays the role of an imaginary time.*

Finally, it is clear that, although our derivation was explicitly performed for a single particle, both of the analogies are true for an arbitrary number of degrees of freedom (although, as we will see in the next chapter, care must be taken to account for particle statistics). In the next section, we will exploit the Feynman path integral formulation to study the quantum mechanics of a particle in a well.

6.3 Bounces in Particle Mechanics

For particle of mass m moving in a one-dimensional potential we saw previously that in a Euclidean (imaginary time) formulation the quantum mechanical evolution operator or propagator is given by

$$G(x, x'; T) \equiv U(x', T; x, 0) = \int_{x(0)=x, x(T)=x'} Dx(\tau) \exp\left[-\frac{1}{\hbar} S[x(\tau)]\right],$$

where the classical imaginary time or Euclidean action is given by

$$S[x(\tau)] = \int_0^T d\tau \left[\frac{m}{2}\dot{x}^2(\tau) + V[x(\tau)]\right].$$

Here $Dx(\tau)$ denotes integration over all functions $x(\tau)$ obeying the boundary conditions $x(0) = x$, and $x(T) = x'$. Equivalently, if $\bar{x}(\tau)$ is any function obeying the boundary condition, then a general function can be written as

$$x(\tau) = \bar{x}(\tau) + \delta x(\tau), \qquad \delta x(\tau) = \sum_n c_n x_n(\tau),$$

where $\{x_n(\tau)\}$ are a complete set of real orthonormal functions vanishing at the boundaries,

$$\int_0^T d\tau\ x_n(\tau)\ x_m(\tau) = \delta_{mn}, \qquad x_n(0) = x_n(T) = 0.$$

Since the measure or Jacobian can always be fixed by normalisation we will not trouble ourselves with it.

In the semi-classical limit ($\hbar \to 0$) the path integral is dominated by stationary contributions of the action. For simplicity, let us first assume that there is only one such stationary trajectory which we will denote by $\bar{x}(\tau)$. The latter obeys the Euler-Lagrange equation,

$$\frac{\delta S}{\delta \bar{x}} \equiv -m\ddot{\bar{x}} + V'(\bar{x}) = 0. \tag{6.8}$$

Substituting for $\bar{x}(\tau)$ and expanding the action to second order in $\delta x(\tau)$, we obtain

$$S[x(\tau)] = S[\bar{x}(\tau)] + \frac{1}{2}\int d\tau \left[m(\delta\dot{x})^2 + V''(\bar{x})(\delta x)^2\right].$$

Note that, by definition of the stationarity condition, the leading order contribution to the action in $\delta x(\tau)$ vanishes. Thus, if we choose x_n's to be the eigenfunctions of the second variational derivative of S at $\bar{x}$,

$$-m\ddot{x}_n + \frac{d^2V}{dx^2}_{\bar{x}} x_n = \lambda_n x_n, \tag{6.9}$$

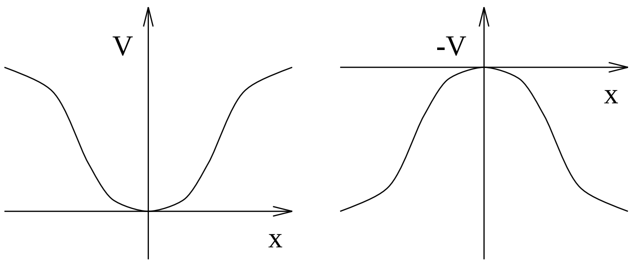

Figure 6.3: Single well (real time) and its inverted counterpart (imaginary time).

the integral becomes a product of Gaussians and we obtain

$$\begin{aligned} G(x,x';T) &= Je^{-S[\bar{x}]}\det\left[-m\partial_t^2+V''(\bar{x})\right]^{-1/2}[1+O(\hbar)] \\ &= Je^{-S[\bar{x}]}\prod_n \lambda_n^{-1/2}[1+O(\hbar)], \end{aligned} \tag{6.10}$$

where J denotes some constant from the measure. More generally, if there are several stationary points, each must be summed separately. We have also tacitly assumed that all the eigenvalues are positive. We will shortly see how to proceed when this isn't the case.

Eq. (6.8) is the equation of motion for a particle of unit mass moving in a potential of *minus* V. Thus

$$E=\frac{m}{2}\dot{\bar{x}}^2-V(\bar{x}),$$

is a constant of the motion. This can be used to determine the qualitative features of the solution by inspection.

As a simple example, consider the potential shown in fig. (6.3). Choosing $x'=x=0$, the inverted potential in fig (6.3) shows that there exists only one solution which obeys the boundary conditions,

$$\bar{x}(\tau)=0.$$

For this solution, $S[\bar{x}]=0$. Setting $V''=m\omega^2$, the infinite product in Eq. (6.10) can be obtained by comparing with the case of the free particle ($\omega=0$),

$$\prod_{n=1}^{\infty}\left(\frac{\lambda_n^{\mathrm{free}}}{\lambda_n}\right)^{1/2}=\left(\prod_{n=1}^{\infty}\frac{1}{1+\omega^2T^2/\pi^2n^2}\right)^{1/2}=\sqrt{\frac{\omega T}{\sinh(\omega T)}}.$$

Thus, using the exact result for the free particle propagator (6.3), we obtain

$$G(0,0;T)=\sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega T)}}[1+O(\hbar)].$$

For a harmonic potential the expansion to second order is exact. In this case it is a straightforward exercise (see problem set III) to obtain the propagator for a more general boundary condition. A general solution to Eq. (6.8) is given by $\bar{x}(\tau) = A\exp(\omega\tau) + B\exp(-\omega\tau)$ where the constant coefficients A and B are determined from the boundary condition $\bar{x}(0) = x$ and $\bar{x}(T) = x'$. From this we obtain

$$S[\bar{x}] = \frac{m\omega}{2}\left([x^2 + x'^2]\coth(\omega T) - \frac{2xx'}{\sinh(\omega T)}\right).$$

In the long time (or low temperature) limit we find

$$\lim_{(\omega T)\to\infty} G(x, x'; T) = \sqrt{\frac{m\omega}{\pi}} e^{-\omega T/2} \exp\left[-\frac{m\omega}{2}(x^2 + x'^2)\right].$$

Comparing with the definition

$$G(x, x'; T) = \sum_m e^{-E_m T/\hbar} \psi_m^*(x)\psi_m(x'),$$

we can deduce that the lowest eigenvalue has the value $E_0 = \hbar\omega/2$ and obtain the ground state wavefunction without solving the Schrödinger equation.

6.4 One-Dimensional Ising Model

The classical one-dimensional Ising model is described by the Hamiltonian

$$-\beta H = \sum_{ij} J_{ij} S_i S_j,$$

where $S_i = \pm 1$ denote single component spins interacting through matrix elements J_{ij}. For ferromagnetic coupling ($J_{ij} > 0$) there exist two degenerate ground state spin configurations in which all spins are aligned along the same direction. A zero temperature there is a spontaneous symmetry breaking in which one ground state is arbitrarily chosen, while at any finite temperature, symmetry is restored by the proliferation of topological defects known as *domain walls* (see fig. 6.4).

6.4.1 Nearest Neighbour Interaction

If the matrix elements couples only neighbouring spins ($J_{ij} = \delta_{i,j\pm 1}/T$) the corresponding partition function can be found exactly and the correlation functions obtained explicitly (either directly from the transfer matrix method or within the block spin RG described problem set II). This is because the energy of some arbitrary spin configuration can be expressed in terms of the number of *domain walls* that separate regions of aligned spins. For N-spins, the partition function is easily shown to be given by

$$\mathcal{Z} = 2\sum_r {}^{N-1}C_r e^{(N-2r)/T},$$

where ${}^{N-1}C_r = (N-1)!/(N-1-r)!r!$ denotes the number of configurations with r domain walls, and the prefactor of two accounts for the degeneracy of the spin configurations in which all spins are reversed.

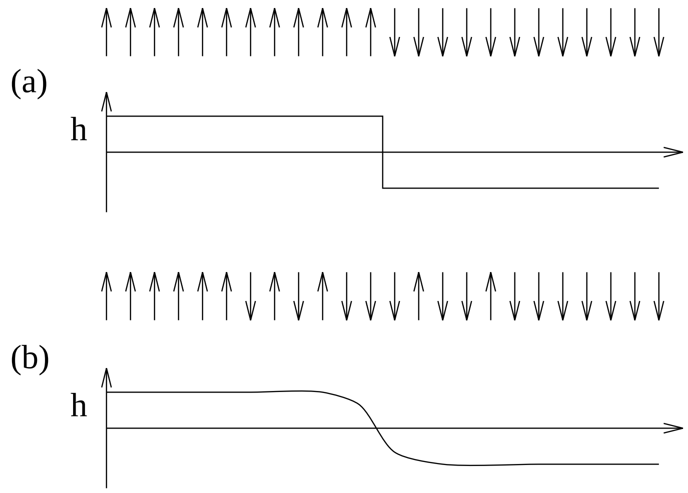

Figure 6.4: Typical spin configurations of the one-dimensional Ising model with (a) a nearest neighbour and (b) a longer range interaction showing a domain wall.

Recognising that the dominant contribution to $\mathcal{Z}$ arises from the interval in which $1 \ll r \ll N$, we can apply Stirling's approximation, ${}^{N-1}C_r \sim N^r/r! \sim N^r \exp[-r\ln(r/e)]$, in which we obtain

$$\mathcal{Z} \sim e^{N/T} \sum_r N^r e^{-2r/T - r\ln(r/e)}.$$

In the mean-field or saddle-point approximation, varying the exponent with respect to r we find that the typical number of domain walls is given by $r^* = N\exp[-2/T]$. Thus, although the typical domain size increases exponentially fast growing as $\exp[2/T]$, in the infinite system a thermodynamic number of domain walls leads to the destruction of long-range order and excludes a phase transition. We can, however, say that it a finite system with N spins, at a temperature "$T_c \sim 2/\ln N$" we would typically expect to find all spins aligned.

Surprisingly a close analogy exists between the statistical mechanics of the one-dimensional Ising model and a quantum mechanical particle confined to a double well. To explore this connection, let us consider a model with a longer-ranged interaction.

6.4.2 Longer-Ranged Interaction

If the interaction between neighbouring spins is long-ranged over a distance $\kappa^{-1} \gg 1$,

$$J_{ij} = \frac{e^{-\kappa|i-j|}}{T},$$

domain walls extend over a large number of lattice sites (see fig. 6.4b). To study the partition function of the corresponding Hamiltonian, it is convenient to recast the model in a "dual" representation by performing a *Hubbard-Stratonovich Transformation.*

In general, any exponential of a quadratic form can be expressed as a Gaussian integral (see Eq. (2.4))

$$\exp\left[\sum_{ij} S_i J_{ij} S_j\right] = C\int_{-\infty}^{\infty}\prod_{k=1}^{N} d\phi_k \exp\left[-\sum_{ij}\phi_i[J^{-1}]_{ij}\phi_j - 2\sum_i S_i\phi_i\right],$$

where for every spin S_i we have introduced a dummy variable ϕ_i, and C denotes an unimportant constant of integration. Substituting this expression into the partition function, and summing over the Ising spins, we obtain

$$\mathcal{Z} = C\int_{-\infty}^{\infty}\prod_{k=1}^{N} d\phi_k \exp\left[-\sum_{ij}\phi_i[J^{-1}]_{ij}\phi_j + \sum_i \ln[2\cosh(2\phi_i)]\right].$$

The inversion of the matrix $\mathbf{J}$ is more readily performed in reciprocal space wherein

$$\sum_{ij} S_i J_{ij} S_j = \int_{-\pi}^{\pi}\frac{dq}{2\pi}J(q)|S(q)|^2, \qquad S_n = \int_{-\pi}^{\pi}\frac{dq}{2\pi}e^{iqn}S(q),$$

with

$$J(q) = \frac{1}{T}\sum_{n=-\infty}^{\infty} e^{inq-\kappa|n|} = \frac{1}{T[c - b\cos(q)]},$$

$c = \coth(\kappa)$ and $b = 1/\sinh(\kappa)$. Using the inverse relation

$$\sum_{ij}\phi_i[J^{-1}]_{ij}\phi_j = \int_{-\pi}^{\pi}\frac{dq}{2\pi}\frac{1}{J(q)}|\phi(q)|^2, \qquad \phi_n = \int_{-\pi}^{\pi}\frac{dq}{2\pi}e^{iqn}\phi(q),$$

we find that

$$\mathbf{J}^{-1} = T\begin{bmatrix} c & -b/2 & 0 & 0 & \cdots \\ -b/2 & c & -b/2 & 0 & \cdots \\ 0 & -b/2 & c & -b/2 & \cdots \\ 0 & 0 & -b/2 & c\cdots & \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}.$$

Altogether, we obtain

$$\mathcal{Z} = C\int\prod_{k=1}^{N} d\phi_k \exp\left[-\frac{bT}{2}\sum_i(\phi_{i+1}-\phi_i)^2 - \sum_i U(\phi_i)\right],$$

where

$$U(\phi) = T(c-b)\phi^2 - \ln[2\cosh(2\phi)], \tag{6.11}$$

and $c - b = \tanh(\kappa/2)$.

In the high temperature phase ($T \gg \kappa^{-1}$) the potential U shows a single minimum at $\phi = 0$ and, as in the nearest neighbour model, the average magnetisation in the

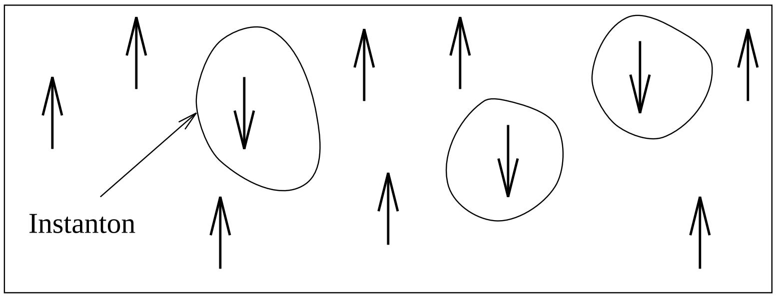

Figure 6.5: Two-dimensional Ising model at low temperatures.

mean-field approximation vanishes. Conversely, in the low temperature phase ($T \ll \kappa^{-1}$) the potential develops two minima at a finite value of ϕ. Thus, within a *mean-field approximation*, Eq. (6.11) implies the existence of a phase transition when

$$t = \left.\frac{\partial^2 U}{\partial \phi^2}\right|_{\phi=0} = 0, \qquad t = 2\left[(c-b)T_c - 2\right] \quad \Longrightarrow \quad T_c = \frac{2}{\tanh(\kappa/2)}.$$

Close to the transition the relevant fluctuations come from long-wavelength modes and justify the continuum limit

$$\mathcal{Z} = \int D\phi \exp\left[-\int d\tau \left(\frac{m}{2}\dot{\phi}^2 + U(\phi)\right)\right], \tag{6.12}$$

where the "mass" $m = bT = T/\sinh(\kappa)$.[3] Just below the transition temperature $T < T_c$, where $(T_c - T)/T_c \ll 1$, $U(\phi)$ can be expanded in the vicinity of the potential minima.

$$U = \frac{t}{2}\phi^2 + \frac{4}{3}\phi^4.$$

A straightforward calculation shows that minima occur at $\phi_*^2 = -3t/16$.

The correspondence between this expression for the partition function and the imaginary time quantum mechanical propagator for a particle in potential double well $U(\phi)$ was first documented in a classic paper by Vaks and Larkin (Sov. Phys. JETP, **22**, 678 (1976)). The restoration of symmetry at any finite temperature can therefore be ascribed to the existence of non-trivial instanton configurations which connect degenerate vacua.

In the case of the two-dimensional Ising model the situation is different. At low temperatures there are random regions of reversed spins (see fig. 6.5). However, since these random fields are short-ranged they do not spoil the correlation and, therefore, the long-range order.

[3]It is left as an exercise to generalised this approach to d-dimensional lattices (see Part III Mathematics Tripos 1997).