# Chapter 6

# Quantum Phase Transitions

*The aim of this chapter is to introduce the Feynman path integral as a useful tool in deriving the Ginzburg-Landau action for a quantum Hamiltonian. We then look at finite-size corrections to RG scaling in order to demonstrate the key ideas behind quantum-classical crossover.*

## 6.1 Path Integral Representation of a Quantum Partition Function

We will be looking at $N$-body quantum Hamiltonians of the form

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \hat{V}(\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, ..., \hat{\mathbf{x}}_N), \tag{6.1}$$

where $\hat{V}(\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, ..., \hat{\mathbf{x}}_N)$ is a many-body potential that generically includes external forces, as well as interactions between particles. $\hat{\mathbf{p}}_i$ and $\hat{\mathbf{x}}_i$ are the momentum and position operators of the $i$th particle and satisfy the usual commutation relations

$$[\hat{x}_\nu, \hat{p}_\mu] = i\delta_{\mu\nu}, \tag{6.2}$$

where $\mu, \nu$ label the $d$ Cartesian components of the operators, and $d$ is the dimensionality. Note that operators corresponding to different particles commute.

The partition function for the Hamiltonian in Eq. 6.1 can be written down in a path integral form using a prescription originally due to Feynman:

$$\mathcal{Z} = \int \left( \prod_{i=1}^{N} d^d\mathbf{x}_i \right) \langle \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N | e^{-\beta \hat{H}} | \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N \rangle. \tag{6.3}$$

To simplify the notation, we will use the following shorthand for both $\mathbf{x}$ and $\mathbf{p}$:

$$
\begin{aligned}
X &\equiv \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N \\
dX &\equiv \left( \prod_{i=1}^{N} d^d \mathbf{x}_i \right), \\
X^2 &\equiv \sum_{i=1}^{N} \mathbf{x}^2, \\
X \cdot P &\equiv \sum_{i=1}^{N} \mathbf{x}_i \cdot \mathbf{p}_i \, .
\end{aligned}
$$

We insert the following resolution of the identity in $N_\tau - 1$ places in the partition function indicated below:

$$
\mathbf{1} = \int dX |X\rangle\langle X| \tag{6.4}
$$

$$
\mathcal{Z} = \int dX \langle X| e^{-\frac{\beta}{N_\tau}\hat{H}} \mathbf{1} e^{-\frac{\beta}{N_\tau}\hat{H}} \mathbf{1} e^{-\frac{\beta}{N_\tau}\hat{H}} ... e^{-\frac{\beta}{N_\tau}\hat{H}} |X\rangle. \tag{6.5}
$$

As $N_\tau \to \infty$, we can expand the exponentials to obtain

$$
\begin{aligned}
\mathcal{Z} = \int \left( \prod_{i=1}^{N_\tau} dX_i \right) &\langle X_1 | \mathbf{1} \left( 1 - \epsilon \hat{H} \right) |X_2\rangle \langle X_2| \mathbf{1} \left( 1 - \epsilon \hat{H} \right) |X_3\rangle \times \\
&\langle X_3 | \mathbf{1} \left( 1 - \epsilon \hat{H} \right) |X_4\rangle \times ... \times \langle X_{N_\tau} | \mathbf{1} \left( 1 - \epsilon \hat{H} \right) |X_1\rangle,
\end{aligned} \tag{6.6}
$$

where $\epsilon = \frac{\beta}{N_\tau}$ and the variable $X$ corresponding to the $(i-1)$th resolution of the identity has been indexed as $X_i$. We now insert the resolution of the identity in momentum space $\mathbf{1} = \int dP |P\rangle\langle P|$ in $N_\tau$ places indicated above to obtain

$$
\begin{aligned}
\mathcal{Z} = \int \left( \prod_{i=1}^{N_\tau} dX_i \right) \int \left( \prod_{i=1}^{N_\tau} dP_i \right) &\langle X_1 | P_1 \rangle \langle P_1 | \left( 1 - \epsilon \hat{H} \right) |X_2\rangle \times \\
\langle X_2 | P_2 \rangle \langle P_2 | \left( 1 - \epsilon \hat{H} \right) |X_3\rangle \times ... \times &\langle X_{N_\tau} | P_{N_\tau} \rangle \langle P_{N_\tau} | \left( 1 - \epsilon \hat{H} \right) |X_1\rangle.
\end{aligned} \tag{6.7}
$$

Using the fact that

$$
\begin{aligned}
\langle X_i | P_j \rangle &= e^{i X_i \cdot P_j}, \\
\langle P_i | \left( 1 - \epsilon \hat{H} \right) |X_{i+1}\rangle &= \left[ 1 - \epsilon \left( \frac{P_i^2}{2m} + V(X_{i+1}) \right) \right] e^{-i P_i \cdot X_{i+1}} \\
&= e^{-\epsilon \left( \frac{P_i^2}{2m} + V(X_{i+1}) \right)} e^{-i P_i \cdot X_{i+1}},
\end{aligned} \tag{6.8}
$$

we obtain the following expression for the partition function valid in the limit $N_\tau \to \infty$:

$$\boxed{\mathcal{Z} = \int \left(\prod_{i=1}^{N_\tau} dX_i\right) \int \left(\prod_{i=1}^{N_\tau} dP_i\right) e^{-i\sum_{i=1}^{N_\tau} P_i\cdot(X_{i+1}-X_i)-\epsilon\sum_{i=1}^{N_\tau}\left(\frac{P_i^2}{2m}+V(X_i)\right)},} \tag{6.9}$$

where $X_{N_\tau+1} = X_1$. The partition function is particularly useful in the continuum limit $X_i \to X(\tau)$, with $\tau = (i-1)\epsilon$, where it becomes a functional integral,

$$\boxed{\mathcal{Z} = \int_{X(\beta)=X(0)} \mathcal{D}X(\tau) \int \mathcal{D}P(\tau) e^{-\int_0^\beta d\tau\left(iP(\tau)\cdot\partial_\tau X(\tau)+\frac{P^2}{2m}+V[X(\tau)]\right)}.} \tag{6.10}$$

Only terms to first order in $\epsilon$ have been kept. Integrating out the momentum fields $P(\tau)$, we obtain the following partition function and a corresponding real action

$$\boxed{\begin{aligned} \mathcal{Z} &= \int_{\mathbf{x}_i(\beta)=\mathbf{x}_i(0)} \mathcal{D}\mathbf{x}_i(\tau) e^{-H[\mathbf{x}_i(\tau)]}, \\ H[\mathbf{x}_i(\tau)] &= \int_0^\beta d\tau \left[\sum_{i=1}^{N} \frac{m|\partial_\tau \mathbf{x}_i|^2}{2} + V[\mathbf{x}_i(\tau)]\right]. \end{aligned}} \tag{6.11}$$

From the form of the partition function above, we see that a $d$-dimensional quantum system at zero temperature $\beta = \infty$ can be mapped onto a $d+1$-dimensional classical system whose energy is given by the classical Hamiltonian and where the extra dimension is spanned by the imaginary time coordinate $\tau$.

A $d$-dimensional quantum system at finite temperature $\beta^{-1}$ can be mapped onto a $(d+1)$- dimensional classical system with the extra dimension now being of finite length $\beta$.

We now turn to analysing particular choices of many-body quantum Hamiltonians that are both illustrative and ubiquitous in condensed matter systems.

**Key correspondences of the Quantum-Classical mapping**

| Correspondence | Quantum | Classical |
|---|---|---|
| Hamiltonian<br>$\hat{H} \leftrightarrow \beta H$ | $\hat{H} = \sum_i \frac{\hat{p}_i^2}{2M} + V[\hat{x}_i]$,<br>where $[\hat{x}_i, \hat{p}_j] = i\delta_{ij}$ | $\beta H = \int_0^\beta \mathrm{d}\tau \left[ \sum_i \frac{M}{2} \left( \frac{\partial m_i(\tau)}{\partial \tau} \right)^2 + V[m_i(\tau)] \right]$ |
| Order Parameter<br>$\hat{x}_i \leftrightarrow m_i(\tau)$ | $\hat{x}_i$ | $m_i(\tau)$ |
| Partition function<br>$\mathcal{Z}_\mathrm{Q} = \mathcal{Z}_\mathrm{C}$ | $\mathcal{Z}_\mathrm{Q} = \sum_n \langle n \vert e^{-\beta \hat{H}} \vert n \rangle$ | $\mathcal{Z}_\mathrm{C} = \int_{m_i(0)=m_i(\beta)} \mathcal{D}m_i(\tau)\; e^{-\beta H[m_i(\tau)]}$ |
| Expectation Value<br>$\langle \hat{x}_i \rangle = \langle m_i(0) \rangle$ | $\langle \hat{x}_i \rangle = \frac{1}{\mathcal{Z}_\mathrm{Q}} \sum_n \langle n \vert e^{-\beta \hat{H}} \hat{x}_i \vert n \rangle$ | $\langle m_i(0) \rangle = \frac{1}{\mathcal{Z}_\mathrm{C}} \int_{m_i(0)=m_i(\beta)} \mathcal{D}m_i(\tau)\; m_i(0) e^{-\beta H[m_i(\tau)]}$ |
| Correlator<br>$\langle e^{\hat{H}\tau} \hat{x}_j e^{-\hat{H}\tau} \hat{x}_i \rangle = \langle m_j(\tau) m_i(0) \rangle$,<br>where $\tau > 0$ | $\langle e^{\hat{H}\tau} \hat{x}_j e^{-\hat{H}\tau} \hat{x}_i \rangle =$<br>$\frac{1}{\mathcal{Z}_\mathrm{Q}} \sum_n \langle n \vert e^{-\beta \hat{H}} e^{\hat{H}\tau} \hat{x}_j e^{-\hat{H}\tau} \hat{x}_i \vert n \rangle$ | $\langle m_j(\tau) m_i(0) \rangle =$<br>$\frac{1}{\mathcal{Z}_\mathrm{C}} \int_{m_i(0)=m_i(\beta)} \mathcal{D}m_i(\tau)\; m_j(\tau) m_i(0) e^{-\beta H[m_i(\tau)]}$ |

**Notes:**

- At zero temperature ($\beta = \infty$), the $\tau$ dimension becomes of infinite extent in the classical picture, and we are integrating over the whole $\tau$-space $\int_0^\beta \mathrm{d}\tau \to \int_{-\infty}^{\infty} \mathrm{d}\tau$. In the quantum picture, the zero-temperature expectation values are taken with respect to the ground state of $\hat{H}$, e.g., $\langle \hat{x}_i \rangle = \frac{1}{\mathcal{Z}_\mathrm{Q}} \langle \mathrm{g.s.} \vert \hat{x}_i \vert \mathrm{g.s.} \rangle$, where $\mathcal{Z}_\mathrm{Q} = \langle \mathrm{g.s.} \vert \mathrm{g.s.} \rangle$.
- In the continuum limit, as usual, the lattice sums are replaced with integrals $\sum_i \to \int \mathrm{d}^d \mathbf{r} / a^d$ and the Kronecker delta with the Dirac delta-function. The commutator $[\hat{x}_i, \hat{p}_j] = i\delta_{ij}$ is replaced with $[\hat{x}(\mathbf{r}), \hat{p}(\mathbf{r}')] = i a^d \delta(\mathbf{r} - \mathbf{r}')$.
- We have assumed translational invariance in $\tau$-space
- Note that the UV cutoff for the imaginary time dimension is $\Lambda_\tau = \infty$. When doing momentum-shell RG this allows us to rescale $\omega$ without changing the cutoff.

## 6.2 O(2) Quantum Rotors

Let us begin by considering the case of a particle constrained to move on a ring of unit radius, centred on the $z$-axis. The particle represents the motion of a 2d rotor of inertia $m$. The 2-dimensional rotor is also known as the O(2) rotor because its possible orientations, described by the unit vector $\mathbf{x} = (\cos\phi, \sin\phi)$, are generated by the O(2) group. The kinetic energy operator of the quantum rotor is given by $\frac{\hat{L}^2}{2m}$, where $\hat{L} = -i\frac{\partial}{\partial_\phi}$ is the $z$ angular momentum operator, i.e., it is the kinetic energy operator of a particle constrained to move on a ring.

We will consider a system of interacting quantum rotors on a $d$-dimensional simple cubic lattice. The rotors interact with their nearest neighbours via a potential of the form $\hat{V}(\hat{\mathbf{x}}_i, \hat{\mathbf{x}}_i) = -g\hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j$. The O(2) quantum rotor Hamiltonian can be written as

$$\boxed{\hat{H}_{\mathrm{O}(2)} = \sum_i \frac{\hat{L}_i^2}{2m} - g\sum_{\langle ij\rangle} \hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j,} \tag{6.12}$$

where $\langle ij\rangle$ indicates that the sum is taken over nearest neighbours only.

**Quantum Phase Transition:** Defined as non-analytic behaviour of the ground state energy of the infinite system. This is therefore a phase transition that takes place at zero temperature.

**Ground state:** The Hamiltonian has a qualitatively different ground state in the large $mg \gg 1$ and low $mg \ll 1$ limits and from this we can infer the presence of a *quantum* phase transition at some intermediate value of $mg$. In the former limit, the potential energy term dominates and rotor alignment is favoured. The second term can be expanded in the rotor azimuthal angle $\hat{\phi}$. The fluctuations will be small and of long-wavelength with a gapless excitation spectrum. The Hamiltonian can be approximated by a series of simple Harmonic oscillators

$$\hat{H} \overset{mg\gg 1}{\approx} \sum_{\mathbf{k}} \left[\frac{1}{2m}\hat{L}_{\mathbf{k}}\hat{L}_{-\mathbf{k}} + \frac{1}{2}g|\mathbf{k}|^2\hat{\phi}_{\mathbf{k}}\hat{\phi}_{-\mathbf{k}}\right], \tag{6.13}$$

where $\hat{\phi}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_i \hat{\phi}_i e^{iki}$ and $\hat{L}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_i \hat{L}_i e^{iki}$ are the Fourier transforms of the operators $\hat{\phi}_i$ and $\hat{L}_i$ respectively. Comparison with the simple harmonic oscillator Hamiltonian shows that the excitation spectrum is given by $\sqrt{\frac{g}{m}}|\mathbf{k}|$.

In the low $mg \ll 1$ limit, the former term dominates and the ground state is given by the zero angular momentum sector for all rotors. The second term can be treated as a perturbation which gives a small (in $mg$) mixing of states. There is therefore an energy gap between the ground state and the first excited state in this phase. We will now look in more detail at the stability of these phases and the transition between them by exploiting the quantum-classical mapping.

The above Hamiltonian is equivalent to the one in Eq. (6.1), provided we choose an additional external potential in Eq. (6.1) that constrains the motion of each particle to a ring. We can therefore immediately write down the corresponding partition function using Eq. (6.11):

$$\boxed{\begin{aligned}\mathcal{Z}_{\mathrm{O}(2)} &= \int\limits_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) e^{-H[\phi_i(\tau)]}, \\ H[\phi_i(\tau)] &= \int_0^\beta d\tau \left[\sum_{i=1}^{N} \frac{m(\partial_\tau \phi_i)^2}{2} - g \sum_{<ij>} \cos(\phi_i - \phi_j)\right],\end{aligned}} \tag{6.14}$$

where $\phi_i$ is the azimuthal angle of the $i$th rotor and is allowed to wind by a multiple of $2\pi$ for the periodic boundary conditions along imaginary time $\tau$.

**Ginzburg-Landau Action**: We proceed to derive the coarse-grained Ginzburg-Landau action for the O(2) quantum rotor Hamiltonian. Its form can be deduced from general symmetries. However, in dimensions $d = 3$ and higher of the Hamiltonian in Eq. (6.12) ($d = 4$ of the corresponding classical action in Eq. (6.14)), where as we will see mean-field behaviour holds well, one might be interested in the bare parameters of the Ginzburg-Landau action. The derivation here mirrors the one for the Ising model.

*Step 1 — Hubbard-Stratonovich decoupling introduces the order parameter:*

$$\begin{aligned}\mathcal{Z}_{\mathrm{O}(2)} &= \mathcal{N} \int\limits_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau)\mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right) e^{-S[\phi_i(\tau),\Psi_i(\tau)]}, \\ S[\phi_i(\tau), \Psi_i(\tau)] &= \int_0^\beta d\tau \sum_i \left\{ \frac{m}{2}(\partial_\tau \phi_i)^2 + \left[e^{i\phi_i(\tau)}\Psi_i(\tau) + e^{-i\phi_i(\tau)}\Psi_i^*(\tau)\right] \right. \\ &\quad \left. + \sum_j \Psi_i^*(\tau) G_{ij}^{-1} \Psi_j(\tau) \right\},\end{aligned} \tag{6.15}$$

where $G_{ij} = \frac{g}{2}$ for nearest neighbours and vanishes otherwise. $\mathcal{N}$ is a normalisation constant and the integration measure $\mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right)$ shows that we are integrating over the real and imaginary parts of the order parameter.

> **Exercise for the Reader:**
> Show by completing the square that integrating out the order parameter $\Psi_i(\tau)$ gives the partion function in Eq. (6.14). Find the required normalisation constant $\mathcal{N}$. *Hint: $\Psi_i(\tau)$ and $\Psi_i^*(\tau)$ can be transformed independently.*

*Step 2 — Expansion in the order parameter:*

$$\mathcal{Z}_{\mathrm{O}(2)} \approx \mathcal{N}\mathcal{Z}_\phi \int \mathcal{D}\left(\Psi_i(\tau),\Psi_i^*(\tau)\right)\Big[1+\sum_i \int d\tau d\tau' \Psi_i(\tau)\Psi_i^*(\tau')\langle e^{i\phi_i(\tau)-i\phi_i(\tau')}\rangle_{S[\phi_i(\tau)]}$$
$$+\frac{12}{4!}\sum_{i\neq j}\int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)+i\phi_j(\tau_3)-i\phi_j(\tau_4)}\rangle_{S[\phi_i(\tau)]}\Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_j(\tau_3)\Psi_j^*(\tau_4)$$
$$+\frac{6}{4!}\sum_i \int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)+i\phi_i(\tau_3)-i\phi_i(\tau_4)}\rangle_{S[\phi_i(\tau)]}\Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_i(\tau_3)\Psi_i^*(\tau_4)\Big]$$
$$\times \exp\left[-\int_0^\beta d\tau \sum_{i,j}\Psi_i^*(\tau)G_{ij}^{-1}\Psi_j(\tau)\right], \quad (6.16)$$

where

$$\mathcal{Z}_\phi \equiv \int_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau)e^{-\int_0^\beta \sum_i \frac{m}{2}(\partial_\tau\phi_i)^2},$$
$$\langle e^{i\phi_j(\tau_1)-i\phi_j(\tau_2)}\rangle_{S[\phi_i(\tau)]} \equiv \frac{1}{\mathcal{Z}_\phi}\int_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau)e^{-\int_0^\beta d\tau\sum_i \frac{m}{2}(\partial_\tau\phi_i)^2}e^{i\phi_j(\tau_1)-i\phi_j(\tau_2)}$$

and similarly for the other averages with respect to $S[\phi_i(\tau)]$. We have truncated the expansion at the fourth order in $\Psi_i(\tau)$. Note that terms that are not invariant under a phase rotation $\phi(\tau)\to\phi(\tau)+\chi$, where $\chi$ is constant in time, have zero expectation value and are not included.

*Step 3 — Integrating out the original field:*

We are interested in the zero-temperature transition where $\beta\to\infty$ and the boundary conditions $\phi_i(\beta)-\phi_i(0)=2\pi n$ can be neglected. In this case, simple Gaussian integration gives $\langle\phi(\tau)\phi(\tau')\rangle_{S[\phi_i(\tau)]}=\frac{1}{2m}|\tau-\tau'|$ and $\langle e^{i\phi(\tau)-i\phi(\tau')}\rangle_{S[\phi_i(\tau)]}=e^{-\frac{1}{2m}|\tau-\tau'|}$. We can thus write down the quadratic term in Eq. 6.16 as

$$\begin{aligned}\int d\tau_1 d\tau_2\, \Psi_i(\tau_1)\Psi_i^*(\tau_2)\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)}\rangle &= \int d\tau_1 d\tau_2\, \Psi_i(\tau_1)\Psi_i^*(\tau_2)e^{-\frac{1}{2m}|\tau_2-\tau_1|}\\
&= \int d\tau du\, \Psi_i(\tau-\frac{u}{2})\Psi_i^*(\tau+\frac{u}{2})\, e^{-|u|/2m}\\
&\approx \int d\tau du\, \left[\Psi_i(\tau)-\frac{u}{2}\partial_\tau\Psi_i(\tau)+\frac{u}{8}\partial_\tau^2\Psi_i(\tau)\right]\\
&\qquad \left[\Psi_i^*(\tau)+\frac{u}{2}\partial_\tau\Psi_i^*(\tau)+\frac{u}{8}\partial_\tau^2\Psi_i^*(\tau)\right]\, e^{-|u|/2m}\\
&= \int d\tau du\, \left[|\Psi_i(\tau)|^2-\frac{u^2}{2}|\partial_\tau\Psi_i(\tau)|^2\right] e^{-|u|/2m}\\
&= \int d\tau\, \left[4m|\Psi_i(\tau)|^2-16m^3|\partial_\tau\Psi_i(\tau)|^2\right], \quad (6.17)\end{aligned}$$

where irrelevant higher order derivatives have been neglected, and we performed integrations by parts and discarded the vanishing boundary terms.

To obtain the coefficients of the quartic terms we need to evaluate the 4-point correlator. In the case $i \neq j$, the four-point correlator reduces to a product of 2-point correlators $\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)}\rangle_{S[\phi_i(\tau)]}\langle e^{i\phi_j(\tau_3)-i\phi_j(\tau_4)}\rangle_{S[\phi_i(\tau)]}$, and we obtain

$$\begin{aligned}
&\frac{1}{2}\sum_{i\neq j}\int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \,\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)}\rangle\langle e^{i\phi_j(\tau_3)-i\phi_j(\tau_4)}\rangle \Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_j(\tau_3)\Psi_j^*(\tau_4)\\
&=\frac{1}{2}\sum_{i\neq j}\left(\int d\tau(4m)|\Psi_i(\tau)|^2\right)\left(\int d\tau(4m)|\Psi_j(\tau)|^2\right), \qquad (6.18)
\end{aligned}$$

where we have used the result of Eq. 6.17 and neglected irrelevant terms of the order of $\Psi^3(\partial\Psi/\partial\tau)$.

The case $i = j$ requires a bit more thought. Here, it is very insightful to map the 4-point path-integral correlator to the expectation value of a quantum operator, although the following can also be derived by Gaussian integration, which the reader is encouraged to do. The derivation of the path integral representation of the quantum partition function in Eq. (6.14) can be straightforwardly extended to find a path integral representation of imaginary time quantum correlators. In general, for an $n$-point correlator, we have

$$\boxed{\begin{aligned}
&\langle A_n(\tau_n)...A_1(\tau_1)\rangle_S \equiv \sum_n \langle n|e^{-\beta\hat{H}}\hat{\mathcal{T}}\left[\hat{A}_n(\tau_n)...\hat{A}_1(\tau_1)\right]|n\rangle,\\
&\hat{A}(\tau) := e^{\hat{H}\tau}\hat{A}e^{-\hat{H}\tau},
\end{aligned}} \qquad (6.19)$$

where $\hat{\mathcal{T}}$ is a time-ordering operator that puts the operators in order of increasing time, starting from the right, $|n\rangle$ are any orthonormal basis vectors and $S$ is the classical action corresponding to the quantum Hamiltonian $\hat{H}$. We can thus write down the 4-point correlator as

$$\begin{aligned}
&\langle e^{i\phi_i(\tau_4)-i\phi_i(\tau_3)+i\phi_i(\tau_2)-i\phi_i(\tau_1)}\rangle_{S[\phi_i(\tau)]} \equiv \langle 0|\hat{\mathcal{T}}\left[e^{i\hat{\phi}_i(\tau_4)}e^{-i\hat{\phi}_i(\tau_3)}e^{i\hat{\phi}_i(\tau_2)}e^{-i\hat{\phi}_i(\tau_1)}\right]|0\rangle,\\
&e^{i\hat{\phi}_i(\tau)} = e^{\hat{H}_0\tau}e^{i\hat{\phi}_i}e^{-\hat{H}_0\tau}, \qquad (6.20)
\end{aligned}$$

where $\hat{H}_0 = \sum_i \frac{\hat{L}_z^2}{2m}$ and $|0\rangle$ is its zero angular momentum ($m_l = 0$) ground state. The operators $e^{\pm\phi_i}$ increase or decrease $m_l$, the $z$ component of angular momentum on site $i$ respectively, by an integer unit. Thus $e^{\pm i\hat{\phi}(\tau)}$ increases/decreases $m_l$ by 1 at time $\tau$. This corresponds to an excitation of the ground state. If we let $m_l(\tau)$ be the angular momentum at time $\tau$, the 4-point correlator can be expressed as follows

$$\langle e^{i\phi_i(\tau_4)-i\phi_i(\tau_3)+i\phi_i(\tau_2)-i\phi_i(\tau_1)}\rangle_{S[\phi_i(\tau)]} = \exp\left[\frac{1}{2m}\int d\tau\, m_l(\tau)^2\right], \qquad (6.21)$$

where $m_l(0) = m_l(\beta) = 0$ and the Boltzmann weight measures the energy cost of the excitations.

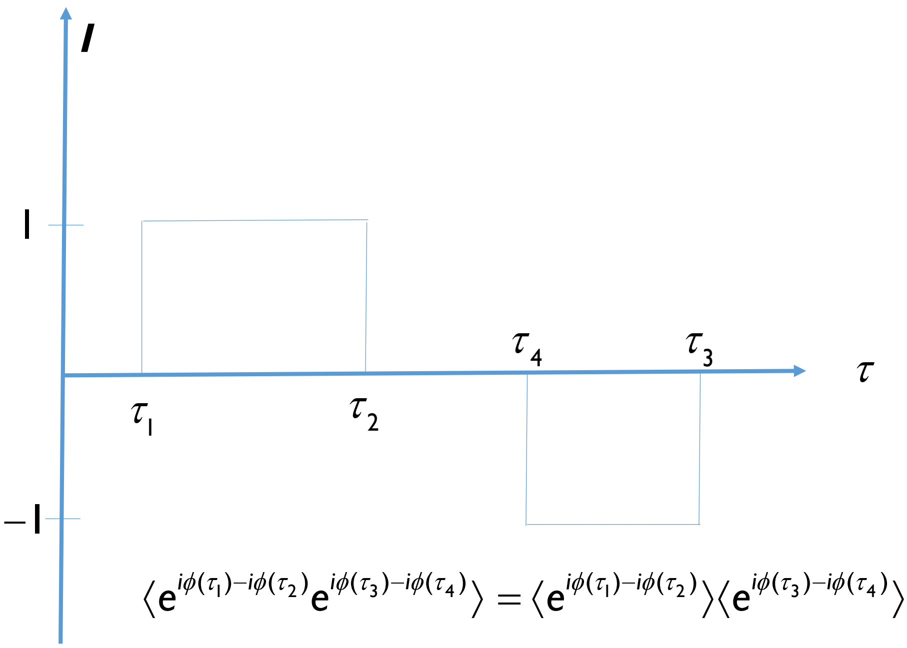


Figure 6.1: The 4-point correlator reduces to a product of 2-point correlators if the $|m_l| \leq 1$ for all imaginary time.

The configurations that we sum over in the penultimate line of Eq. 6.16 fall into two categories:

- (a) $|m_l(\tau)| \leq 1$, $\forall \tau$.

  In this case the 4-point correlator can always be expressed as a product of two *non-overlapping* 2-point correlators. See Fig. 6.1 for an example. The two $|m_l| = 1$ excitations (one for each 2-point correlator) can be translated freely in time with no change in the energy cost as long as they do not overlap.

  To sum over all configurations, we take the ordering $\tau_{1,2} < \tau_{3,4}$ without loss of generality. Remember that the raising operators act at times $\tau_1$ and $\tau_3$ and the lowering operators at times $\tau_2$ and $\tau_4$. There are $2^2$ equivalent orderings that preserve the constraint $|m_l(\tau)| \leq 1$, $\forall \tau$ obtained by the independent interchanges

$\tau_1 \leftrightarrow \tau_3$ and $\tau_2 \leftrightarrow \tau_4$:

$$
\begin{aligned}
&\frac{2^2}{4}\int\limits_{\tau_{1,2}<\tau_{3,4}} d\tau_1 d\tau_2 d\tau_3 d\tau_4\ \Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_i(\tau_3)\Psi_i^*(\tau_4)\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)+i\phi_i(\tau_3)-i\phi_i(\tau_4)}\rangle = \\
&\int\limits_{t_2-t_1>\frac{|u_1|+|u_2|}{2}} du_1du_2dt_1dt_2\ \Psi_i(t_1-\frac{u_1}{2})\Psi_i^*(t_1+\frac{u_1}{2})\Psi_i(t_2-\frac{u_2}{2})\Psi_i^*(t_2+\frac{u_2}{2}) \\
&\qquad\qquad\times e^{-|u_1|/2m-|u_2|/2m} \\
&\approx \int\limits_{t_2-t_1>\frac{|u_1|+|u_2|}{2}} du_1du_2dt_1dt_2\ |\Psi_i(t_1)|^2|\Psi_i(t_2)|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&= \int\limits_{u>\frac{|u_1|+|u_2|}{2}} du_1du_2d\tau du\ |\Psi_i(\tau-\frac{u}{2})|^2|\Psi_i(\tau+\frac{u}{2})|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&= \frac{1}{2}\int du_1du_2d\tau du\ |\Psi_i(\tau-\frac{u}{2})|^2|\Psi_i(\tau+\frac{u}{2})|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&-\frac{1}{2}\int\limits_{|u|<\frac{|u_1|+|u_2|}{2}} du_1du_2d\tau du\ |\Psi_i(\tau-\frac{u}{2})|^2|\Psi_i(\tau+\frac{u}{2})|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&\approx \frac{1}{2}\int dt_1dt_2\ |\Psi_i(t_1)|^2|\Psi_i(t_2)|^2(4m)^2 \\
&-\frac{1}{2}\int du_1du_2d\tau\ |\Psi_i(\tau)|^4\left(|u_1|+|u_2|\right)e^{-|u_1|/2m-|u_2|/2m} \\
&\approx \frac{1}{2}\left(\int d\tau\ 4m|\Psi_i(\tau)|^2\right)^2 - 32m^3\int d\tau\ |\Psi_i(\tau)|^4, \qquad (6.22)
\end{aligned}
$$

where $t_1 = (\tau_1+\tau_2)/2$, $u_1 = (\tau_2-\tau_1)$, $t_2 = (\tau_3+\tau_4)/2$, $u_2 = (\tau_4-\tau_3)$ and $\tau = (t_1+t_2)/2$, $u = (t_2-t_1)$. Irrelevant terms of the order of $\Psi^3(\partial\Psi/\partial\tau)$ have been neglected.

- (b) $|m_l(\tau)| = 2$ for some non-zero time.

If the angular momentum is raised (or lowered) twice before it is lowered (or raised) twice $|m_l| = 2$ for some non-zero time, which carries an increased energy cost. Such configurations cannot be expressed as products of 2-point correlators, but are energetically supressed and do not play a vital role in the quantum phase transition. See Fig. 6.2 for an example.

Again to sum over the relevant configurations, we take the ordering $\tau_{1,3} < \tau_{2,4}$. There are two equivalent orderings, obtained by the simultaneous interchange of

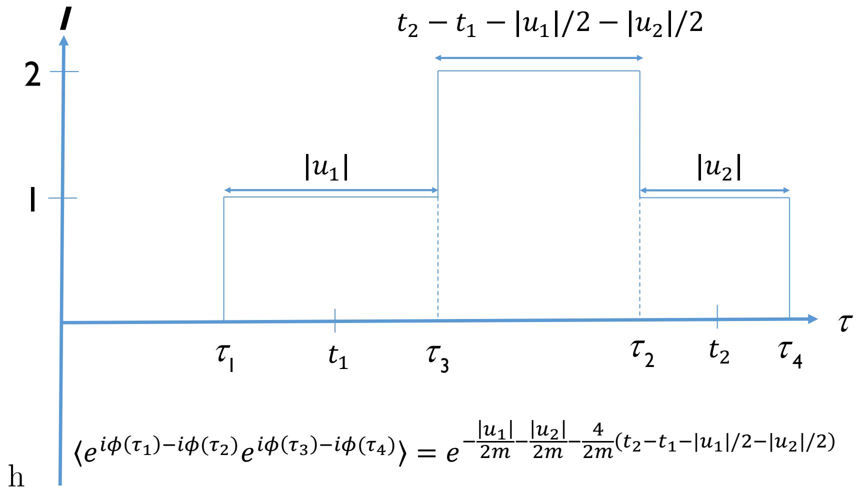


Figure 6.2: The 4-point correlator does not reduce to a product of 2-point correlators if $|m_l| = 2$ for non-zero imaginary time.

$\tau_1 \leftrightarrow \tau_2$ and $\tau_3 \leftrightarrow \tau_4$:

$$
\begin{aligned}
&\frac{2}{4} \int\limits_{\tau_{1,3}<\tau_{2,4}} d\tau_1 d\tau_2 d\tau_3 d\tau_4 \; \Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_i(\tau_3)\Psi_i^*(\tau_4)\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)+i\phi_i(\tau_3)-i\phi_i(\tau_4)}\rangle \\
&= \frac{1}{2} \int\limits_{t_2-t_1>\frac{|u_1|+|u_2|}{2}} du_1 du_2 dt_1 dt_2 \; \Psi_i(t_1-\frac{u_1}{2})\Psi_i(t_1+\frac{u_1}{2})\Psi_i^*(t_2-\frac{u_2}{2})\Psi_i^*(t_2+\frac{u_2}{2}) \\
&\times \exp\left[-\frac{|u_1|}{2m} - \frac{|u_2|}{2m} - \frac{2}{m}\left((t_2-t_1) - \frac{|u_1|}{2} - \frac{|u_2|}{2}\right)\right] \\
&\approx \frac{1}{2}\int d\tau \, |\Psi_i(\tau)|^4 \int\limits_{u>\frac{|u_1|+|u_2|}{2}} du_1 du_2 du \; e^{-2u/m+|u_1|/2m+|u_2|/2m} \\
&= \frac{1}{4}\int d\tau \, |\Psi_i(\tau)|^4 \int du_1 du_2 du \; e^{-2|u|/m-|u_1|/2m-|u_2|/2m} = 4m^3 \int d\tau \, |\Psi_i(\tau)|^4 \,,
\end{aligned}
$$

where $t_1 = (\tau_1 + \tau_3)/2$, $u_1 = (\tau_3 - \tau_1)$, $t_2 = (\tau_2 + \tau_4)/2$, $u_2 = (\tau_4 - \tau_2)$ and $\tau = (t_1 + t_2)/2$, $u = (t_2 - t_1)$. Irrelevant terms of the order of $\Psi^3(\partial\Psi/\partial\tau)$ have been neglected.

Putting everything together, we can write down

$$\mathcal{Z}_{\mathrm{O}(2)} \approx \mathcal{N}\mathcal{Z}_\phi \int \mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right) \left[1 + \sum_i \int d\tau \left(4m|\Psi_i(\tau)|^2 - 16m^3|\partial_\tau \Psi_i(\tau)|^2\right) + \frac{1}{2}\left(\sum_i \int d\tau 4m|\Psi_i(\tau)|^2\right)^2 - 28m^3 \sum_i \int d\tau |\Psi_i(\tau)|^4\right] e^{-\int_0^\beta \sum_{i,j} \Psi_i^*(\tau) G_{ij}^{-1} \Psi_j(\tau)}. \tag{6.23}$$

*Step 4 – Re-expontiation:*

Firstly note that in Fourier space the matrix $G$ is diagonal:

$$G_{\mathbf{q},\mathbf{q}'} = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot\mathbf{x}_i - i\mathbf{q}'\cdot\mathbf{x}_j} G_{ij} = \delta_{\mathbf{q}+\mathbf{q}'} \sum_{\mu=1,\ldots,d} 2g\cos(q_\mu a) = 2g\delta_{\mathbf{q}+\mathbf{q}'}\left[d - |\mathbf{q}|^2\frac{a^2}{2} + \mathcal{O}(|\mathbf{q}|^4)\right], \tag{6.24}$$

and its inverse is given by

$$G^{-1}_{\mathbf{q},\mathbf{q}'} = \delta_{\mathbf{q}+\mathbf{q}'}(2gd)^{-1}\left[1 + \frac{a^2}{2d}|\mathbf{q}|^2 + \mathcal{O}(|\mathbf{q}|^4)\right]. \tag{6.25}$$

Since we are interested in the coarse-grained long-wavelength properties of the system we will only keep the first two terms in the expansion for $G^{-1}_{\mathbf{q},\mathbf{q}'}$.

Coarse-graining the summation over lattice sites $\Psi_i(\tau) \to \Psi(\mathbf{r},\tau)$, $\sum_i \to \int \frac{d^d\mathbf{r}}{a^d}$ and re-expontiating the terms in the square brackets we obtain the final expression for the O(2) quantum rotor Ginzburg-Landau action:

$$\begin{aligned} \mathcal{Z}_{\mathrm{O}(2)} &\approx \mathcal{N}\mathcal{Z}_\phi \int \mathcal{D}\left(\Psi(\mathbf{r},\tau), \Psi^*(\mathbf{r},\tau)\right) e^{-S[\Psi(\mathbf{r},\tau)]}, \\ S[\Psi(\mathbf{r},\tau)] &= \int \frac{d^d\mathbf{r}}{a^d} d\tau \Big[t|\Psi(\mathbf{r},\tau)|^2 + \frac{a^2}{4gd^2}|\nabla\Psi(\mathbf{r},\tau)|^2 \\ &\quad + 16m^3|\partial_\tau\Psi(\mathbf{r},\tau)|^2 + 28m^3|\Psi(\mathbf{r},\tau)|^4\Big] \\ &\quad - \frac{1}{2}\left(\int \frac{d^d\mathbf{r}}{a^d} d\tau 4m|\Psi(\mathbf{r},\tau)|^2\right)^2, \end{aligned} \tag{6.26}$$

where $t = (\frac{1}{2gd} - 4m)$. Note that the $t = 0$ corresponds to the zero-temperature transition, where $g = \frac{1}{8md}$, and $t = -4m$ corresponds to the classical limit, where $g = \infty$. The above derivation makes it clear that proliferation of virtual (in imaginary time) particle-hole excitations $m_l = \pm 1$ drives the quantum phase transition from the gapped phase to the ordered phase. The stability of the Ginzburg-Landau action is ensured by the quartic term, which originates from hardcore repulsion between particle-hole pairs. Virtual particle-hole proliferation is also the mechanism behind the quantum phase transition in the Bose-Hubbard model and there it results in boson condensation. The two are in fact in the same $O(2)$ universality class.

**Dynamical Exponent:** The Ginzburg-Landau action for the quantum O(2) rotor is istropic in spacetime, which can be explicitly shown by rescaling time and space $\mathbf{r} \to \frac{a}{2\sqrt{g}\,d}\mathbf{r}$, $\tau \to \tau 4m^{3/2}$. (In fact the theory is also relativistic with a speed of light equal to unity after rescaling). The correlations in time and space will therefore diverge with the same exponent at the critical point $t = 0$,

$$\xi \sim \xi_\tau \sim \frac{1}{|t|^\nu}. \tag{6.27}$$

This is however generally not the case as question 2 on the second example sheet demonstrates. In general,

$$\boxed{\begin{aligned} \xi &\sim \frac{1}{|t|^\nu}, \\ \xi_\tau &\sim \frac{1}{|t|^{z\nu}}, \end{aligned}} \tag{6.28}$$

where $z$ is known as the dynamical exponent. For O(N) quantum rotor systems, $z = 1$.

**Energy Gap:** A finite energy gap (in the thermodynamic limit, namley as system size tends to infinity) between the lowest excitation and the ground state results in a finite correlation length in imaginary time $\xi_\tau$ for ground state expectation values. From Eq. (6.19) expressed in the energy eigenstates basis $|n\rangle$ and at zero temperature, we obtain

$$\begin{aligned} \langle A(\tau)B(\tau')\rangle_{S[\phi_i(\tau)]} &\equiv \sum_n \langle 0|\hat{A}|n\rangle e^{-|\tau-\tau'|E_n/\hbar}\langle n|\hat{B}|0\rangle \\ &\stackrel{|\tau-\tau'|\to\infty}{\to} \langle 0|\hat{A}|1\rangle e^{-|\tau-\tau'|E_1/\hbar}\langle 1|\hat{B}|0\rangle, \end{aligned} \tag{6.29}$$

where without loss of generality $E_0 = 0$ and $E_1$ is the energy gap to the first excited state, which dominates the sum in the limit $|\tau - \tau'|$. We thus conclude that the imaginary time correlation length $\xi_\tau$ is related to the energy gap to the first excited state as follows:

$$\boxed{\xi_\tau = \frac{\hbar}{E_1}.} \tag{6.30}$$

## 6.3 † O(3) Quantum Rotors

We now consider the case of a particle constrained to move on a sphere of unit radius. The particle represents the motion of a 3D rotor of inertia $m$. The kinetic energy operator of the quantum rotor is given by the kinetic energy operator of a particle constrained to move on a sphere, i.e., $\frac{\hat{\mathbf{L}}^2}{2m}$, where $\hat{\mathbf{L}}$ is the usual angular momentum operator. The

3-dimensional rotor is also known as an O(3) rotor because its possible orientations, described by the unit vector $\mathbf{x}$, are generated by the O(3) group.

As before, we will consider a system of interacting quantum rotors on a $d$-dimensional simple cubic lattice. The rotors interact with their nearest neighbours via a potential of the form $g\hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j$ . The O(3) quantum rotor Hamiltonian can be written as follows

$$\boxed{\hat{H}_{\mathrm{O}(3)} = \sum_i \frac{\hat{\mathbf{L}}_i^2}{2m} - g \sum_{<ij>} \hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j \,.} \tag{6.31}$$

As before, naive expansions lead to the conclusion that there are two zero-temperature phases (i.e., two qualitatively different ground states): an ordered one with gapless excitations, where $\langle \hat{\mathbf{x}} \rangle \neq \mathbf{0}$, at large $mg$; and a disordered one with gapped excitations, where $\langle \hat{\mathbf{x}} \rangle = \mathbf{0}$, at small $mg$.

As before, the above Hamiltonian is equivalent to the one in Eq. (6.1), provided we choose an additional external potential in Eq. (6.1) that constrains the motion of each particle to a sphere and gives rise to a functional delta function in the partition function. It then follows from Eq. (6.11) that the O(3) quantum rotor partition function is given by

$$\boxed{\begin{aligned} \mathcal{Z}_{\mathrm{O}(3)} &= \int\limits_{\mathbf{x}_i(\beta)=\mathbf{x}_i(0)} \mathcal{D}\mathbf{x}_i(\tau)\, \delta\left(\mathbf{x}^2 - 1\right) e^{-H[\mathbf{x}_i(\tau)]}, \\ H[\mathbf{x}_i(\tau)] &= \int_0^\beta d\tau \left[ \sum_{i=1}^N \frac{m(\partial_\tau \mathbf{x}_i)^2}{2} - g \sum_{<ij>} \mathbf{x}_i . \mathbf{x}_j \right] . \end{aligned}} \tag{6.32}$$

**Weak coupling limit and the non-linear $\sigma$ model:** As before, we could proceed to derive the Ginzburg-Landau action or simply write it down on a phenomenological basis with undetermined parameters. However, we shall be mostly interested in the properties of the model in the limit $mg \gg 1$, also known as the weak coupling limit. The reasons behind this name will soon become apparent. When $mg \gg 1$, the fluctuations in $\mathbf{x}_i(\tau)$ will involve only long wavelength modes which can be treated in a continuum approximation. Accordingly, we can make the replacement

$$\begin{aligned} -g \sum_{<ij>} \mathbf{x}_i(\tau) \cdot \mathbf{x}_j(\tau) &= \frac{g}{2} \sum_{<ij>} \left[\mathbf{x}_i(\tau) - \mathbf{x}_j(\tau)\right]^2 + \text{const.} \\ &\to \frac{g}{2} \int \frac{d^d\mathbf{r}}{a^{d-2}} |\nabla \mathbf{S}(\mathbf{r},\tau)|^2, \end{aligned} \tag{6.33}$$

where we have replaced the lattice variables $\mathbf{x}_i(\tau)$ with the continuous vector field $\mathbf{S}(\mathbf{r},\tau)$. Rescaling time and space $\tau \to \tau\sqrt{\frac{m}{2}}$, $\mathbf{r} \to \mathbf{r}\sqrt{\frac{ga}{2}}$, we obtain the non-linear $\sigma$ model:

$$\boxed{\begin{aligned} \mathcal{Z} &= \int \mathcal{D}\mathbf{S}(\mathbf{r},\tau)\delta(\mathbf{S}\left(\mathbf{r},\tau\right)^2 - 1)e^{-S[\mathbf{S}(\mathbf{r},\tau)]}, \\ S[\mathbf{S}(\mathbf{r},\tau)] &= \frac{1}{f} \int \frac{d^d\mathbf{r}d\tau}{a^d} \partial_\mu \mathbf{S}(\mathbf{r},\tau)\partial^\mu \mathbf{S}(\mathbf{r},\tau), \end{aligned}} \tag{6.34}$$

where the dimensionful coupling $f = (\frac{4}{g^d a^d m})^{\frac{1}{2}}$. In the weak-coupling limit $mg \gg 1$ the variations in $\mathbf{S}(\mathbf{r},\tau)$ around a globally uniform configuration will be small and we can expand the non-linear $\sigma$ model action as

$$\begin{aligned} S[\mathbf{S}(\mathbf{r},\tau)] &= \frac{1}{f}\int \frac{d^d\mathbf{r}d\tau}{a^d}\left(\mathbf{e}_\theta\partial_\mu\theta + \mathbf{e}_\phi\sin\theta\partial_\mu\phi\right)\cdot\left(\mathbf{e}_\theta\partial_\mu\theta + \mathbf{e}_\phi\sin\theta\partial_\mu\phi\right) \\ &\overset{\theta\to\frac{\pi}{2}+\theta}{=} \frac{1}{f}\int \frac{d^d\mathbf{r}d\tau}{a^d}\left[\partial_\mu\theta\partial^\mu\theta + \partial_\mu\phi\partial^\mu\phi - \frac{1}{2}\theta^2\partial_\mu\phi\partial^\mu\phi + \mathcal{O}(\theta^4\phi^2)\right] \\ &\overset{\substack{\theta\to\sqrt{f}\theta \\ \phi\to\sqrt{f}\phi}}{=} \int \frac{d^d\mathbf{q}d\tau}{(2\pi)^d a^d}\left[|\partial_\tau\theta(\mathbf{q})|^2 + |\partial_\tau\phi(\mathbf{q})|^2 + |\mathbf{q}|^2\left(|\theta(\mathbf{q})|^2 + |\phi(\mathbf{q})|^2\right)\right] \end{aligned} \tag{6.35}$$

where $\theta(\mathbf{r},\tau)$ and $\phi(\mathbf{r},\tau)$ are the spherical polar angles of the spin vector $\mathbf{S}(\mathbf{r},\tau)$, and $\theta = \pi/2$, $\phi = 0$ in the globally uniform configuration around which we are expanding.

Comparison with Eq. (6.11) shows that in the weak-coupling limit the original Hamiltonian can be approximated by a sum of simple harmonic oscillators, one for each mode $\mathbf{q}$ and an interaction that is proportional to the coupling $f$. In quantum field theory language the excitation of the $\mathbf{q}$-mode simple harmonic oscillator corresponds to creating particles with momentum $\hbar\mathbf{q}$, energy $2|\mathbf{q}|$ and the weak interaction that scales with $f$ is responsible for particle-particle scattering.

$$\begin{aligned} \hat{H} &= \int \frac{d^d\mathbf{q}}{(2\pi)^d}\left[\hat{\pi}_\theta(\mathbf{q})\hat{\pi}_\theta(-\mathbf{q}) + \hat{\pi}_\phi(\mathbf{q})\hat{\pi}_\phi(-\mathbf{q}) + |\mathbf{q}|^2\left(\hat{\theta}(\mathbf{q})\hat{\theta}(-\mathbf{q}) + \hat{\phi}(\mathbf{q})\hat{\phi}(-\mathbf{q})\right)\right], \\ &\quad +\mathcal{O}(f) \end{aligned} \tag{6.36}$$

with the canonical commutation relations $[\hat{\pi}_\theta(\mathbf{q}),\hat{\theta}(\mathbf{k})] = \delta_{\mathbf{k}+\mathbf{q}}$ and $[\hat{\pi}_\phi(\mathbf{q}),\hat{\phi}(\mathbf{k})] = \delta_{\mathbf{k}+\mathbf{q}}$.

**Exercise for the Reader:**
Show that the above Hamiltonian does indeed host gapless excitations with energy proportional to $|\mathbf{q}|$.

**Haldane Gap:** Our analysis of the previous chapter showed that in $d = 2$, the Gaussian $f = 0$ fixed point ($T = 0$ of the corresponding classical model) of the $N = 3$ non-linear sigma model is unstable and the model flows towards the phase with a finite correlation length which close to $f = 0$ varies as follows (isotropically along rescaled $\tau$ and $\mathbf{r}$):

$$\xi \sim a e^{\frac{2\pi}{f}}. \tag{6.37}$$

Thus the energy gap $\Delta$ of the corresponding quantum O(3) rotor chain ($d = 1$) is given by

$$\Delta = \frac{1}{\xi} \sim e^{-\frac{2\pi}{f}}. \tag{6.38}$$

The energy gap $\Delta$ is known as the Haldane gap in the context of Heisenberg antiferromagnetic chains with integer spins, which map onto the one-dimensional quantum O(3) rotor chains.

**Asymptotic Freedom:** Following on from our investigation of the 2-dimensional classical non-linear sigma model in the previous Chapter, where we showed that high-momentum correlators are given by a quadratic theory with an effective coupling that vanishes logarithmically as $p \to \infty$, we conclude that the high-momentum, large-energy excitations of the above *quantum field Hamiltonian* interact weakly at large momenta. (At low momenta the interactions are strong since the running coupling grows.) The particles, represented by these excitations, are thus *free* at large momenta and energies. This is known as *asymptotic freedom.* A similar phenomenon occurs in quantum chromodynamics (QCD), where the quarks interact strongly at small energies and are confined to form hadrons but behave as free particles at large energies.

## 6.4 Finite-Size Scaling

In this section we look at finite-size corrections to the critical properties of the $d$-dimensional Ising model with the following Ginzburg-Landau action,

$$S[\Psi(\mathbf{x})] = \int d^d\mathbf{x} \left[ (\nabla\Psi(\mathbf{x}))^2 + t\Psi^2(\mathbf{x}) + u\Psi(\mathbf{x})^4 - h\Psi(\mathbf{x}) \right] , \tag{6.39}$$

although the scalings that we derive are applicable to most critical systems. We consider a system of finite extent, i.e., length $L$ along each dimension. An RG transformation involves the rescaling of each dimension

$$\begin{aligned} \mathbf{x} &= b\mathbf{x}', \\ L &= bL'. \end{aligned} \tag{6.40}$$

We therefore conclude that the inverse system size $L^{-1}$ is a relevant RG variable with eigenvalue $y_{L^{-1}} = 1$

$$\boxed{\begin{aligned} &L'^{-1} = bL^{-1}, \\ &y_{L^{-1}} = 1. \end{aligned}} \tag{6.41}$$

The free energy density changes by a scaling factor (homogeneously) under an RG transformation

$$f\left(t, h, L^{-1}\right) = b^{-d} f\left(b^{y_t}t, b^{y_h}h, bL^{-1}\right) \tag{6.42}$$

where we only need to include relevant variables sufficiently close to the critical point. It follows that the singular part of the susceptibility has the following form

$$\begin{aligned} \chi \sim \frac{\partial^2 f}{\partial h^2}_{h=0} &= b^{2y_h - d} f\left(b^{y_t}t, bL^{-1}\right) \\ &\overset{b^{y_t}t=1}{=} t^{\frac{d-2y_h}{y_t}} \Phi(t^{-\frac{1}{y_t}} L^{-1}) \\ &= t^{-\gamma}\Phi(t^{-\nu}L^{-1}) \\ &= L^{\frac{\gamma}{\nu}}\Psi(\xi L^{-1}), \end{aligned} \tag{6.43}$$

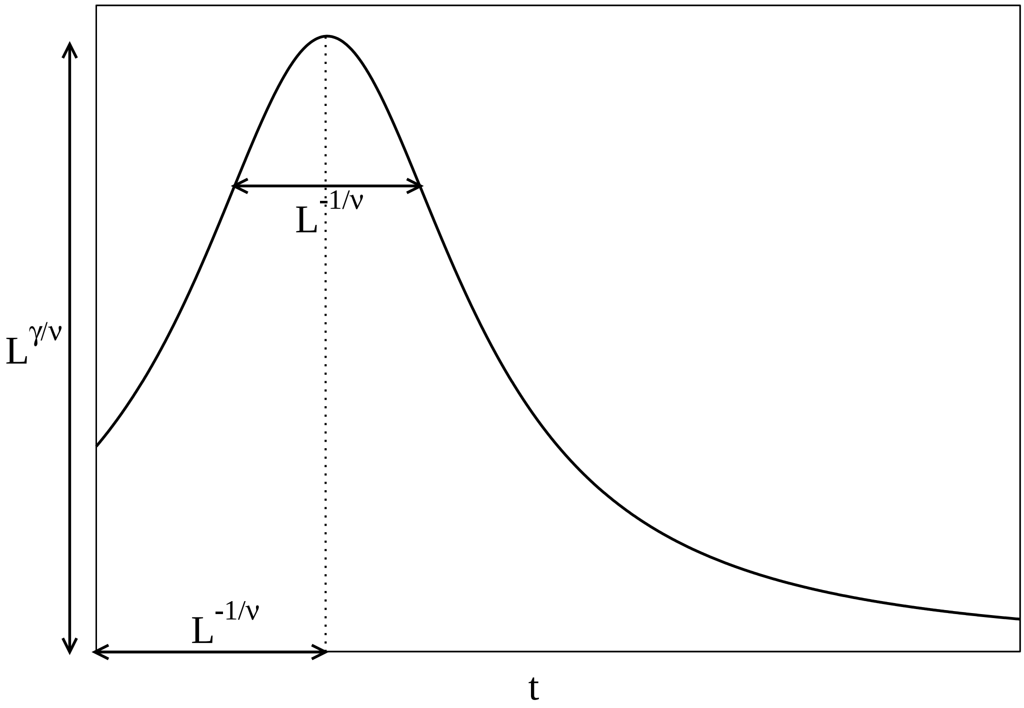


Figure 6.3: Scaling of susceptibility with system size.

where the homogenous function $\Psi(x)$ is a finite function of the order of unity since the susceptibility of a finite system cannot have any singularities. $\Psi(x) \to x^{\frac{\gamma}{\nu}}$ as $x \to 0$ restores the correct universal behaviour in the thermodynamic limit. There is therefore a smooth crossover to the thermodynamic limit behaviour when $\xi L^{-1} \sim \mathcal{O}(1)$, i.e., at a crossover temperature

$$\boxed{t_X = L^{-\frac{1}{\nu}}.} \tag{6.44}$$

The susceptibility of a finite system is still expected to have a finite maximum in the vicinity of the transition point. The function $\Psi(x)$ has a maximum at some value $x \sim \mathcal{O}(1)$ and with a width $\Delta x \sim \mathcal{O}(1)$. We therefore conclude that for finite systems the susceptibility has a maximum at $t \sim L^{-\frac{1}{\nu}}$ with a width $\Delta t \sim L^{-\frac{1}{\nu}}$ and an amplitude that scales as $L^{\frac{\gamma}{\nu}}$. Fig. 6.3 illustrates the main points.

## 6.5 Quantum Critical Behaviour

We will focus on the $d$-dimensional quantum O(2) rotor system with the following Hamiltonian (Eq. (6.12))

$$\boxed{\hat{H}_{\mathrm{O}(2)} = \sum_i \frac{\hat{L}_z^2}{2m} - g \sum_{<ij>} \hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j,} \tag{6.45}$$

and a corresponding classical partition function (Eq. (6.14))

$$\boxed{\begin{aligned} \mathcal{Z}_{\mathrm{O}(2)} &= \int\limits_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) e^{-H[\phi_i(\tau)]}, \\ H[\phi_i(\tau)] &= \int_0^\beta d\tau \left[ \sum_{i=1}^{N} \frac{m(\partial_\tau \phi_i)^2}{2} - g \sum_{<ij>} \cos(\phi_i - \phi_j) \right]. \end{aligned}} \tag{6.46}$$

We take $d > 2$ so that the O(2) rotor system orders at finite temperature. The partition function of the $d$ dimensional quantum system can be written as the partition function of a corresponding $(d+1)$-dimensional classical system. The zero-temperature ($\beta = \infty$) quantum transition maps onto the classical $(d+1)$-dimensional fixed point $F_{d+1}$ with a relevant scaling variable $t = (\frac{1}{g} - 4m)$. The exponents controlling RG flow around this fixed point belong to the $(d+1)$-dimensional $n = 2$ universality class.

We have seen (by deriving the relevant Ginzburg-Landau action) that in the vicinity of the quantum critical point $F_{d+1}$, where the correlation length diverges along the spatial and imaginary time directions, a continuum field-theory picture is valid. The imaginary time dimension enters on the same footing as the spatial dimensions and controls the size of the system. Now, if the quantum system is at a finite-temperature $T$ the extra dimension of the corresponding classical system becomes finite with a length $L = \beta$. Therefore, temperature $T = L^{-1}$ is a relevant RG variable around the $F_{d+1}$ fixed point with eigenvalue $y_T = 1$. Fig. 6.4 shows the RG flow around the $F_{d+1}$ fixed point – the quantum critical point.

The axis $t = -4m$ ($g = \infty$) corresponds to classical $d$-dimensional O(2) rotors and contains the usual stable low and high temperature fixed points corresponding to the ordered and disorderd phases respectively (see the high/low temperature expansions in Chapter 4). These are separated by the $d$-dimensional fixed point $F_d$ at $T = T_c$. The exponents controlling RG flow around $F_{d+1}$ belong to the $n = 2$, $d$-dimensional universality class. Note that $t$ is an irrelevant RG variable at this point, because fluctuations of $\phi_i(\tau)$ along the imaginary time direction $\tau$ are gapped out. $\omega = \frac{2\pi}{\beta}$ is the lowest allowed frequency and $2\pi^2 m T_c \sim 2\pi^2 m g \gg 1$ is the energy cost of this mode ($T_c \sim g$). Also note that the stable Gaussian fixed point at $t = -4m$, $T = 0$, is a terminating point for all RG trajectories inside the ordered phase.

**Quantum-Classical Crossover:** We now employ the finite-size scaling arguments of the preceding section to discuss quantum-classical crossover in the vicinity of the quantum critical point $F_{d+1}$. Using Eq. (6.43) with $L^{-1} = T$ we can express the singular part of the susceptibility in the vicinity of the quantum critical point as

$$\boxed{\chi = T^{-\frac{\gamma}{\nu}} \Psi(T\xi),} \tag{6.47}$$

where $\gamma$ and $\nu$ are the critical exponents associated with the $F_{d+1}$ fixed point. Note that, $\Psi(x) \to x^{\frac{\gamma}{\nu}}$ recovers the correct zero-temperature limit. However, unlike the case of a system of finite extent in all directions, the susceptibility and the function $\Psi(x)$ do not have to be finite for non-zero $T$. In fact, we expect a singularity in $\Psi$ associated with crossing the ordered-disordered phase boundary at some value $T\xi = b \sim \mathcal{O}(1)$. This singularity will be controlled by the critical exponents associated with the $F_d$ fixed point $\gamma'$ and $\nu'$. We can therefore write

$$\boxed{\chi = T^{-\frac{\gamma}{\nu}} (T\xi - b)^{\gamma'} \quad \text{for } T\xi \sim b.} \tag{6.48}$$

The transition temperature scales like $T_c = bt^{\nu}$ in the vicinity of the critical point. Note that the susceptibility is controlled by the above classical $F_d$ singular behaviour for $T\xi \sim b$. This condition maps out the wedge marked in Fig. 6.4 which gets narrower as we approach the quantum critical point. The characteristic cross-over temperature associated with passing between classical $T\xi \sim b$ and quantum $T\xi \ll 1$ behaviour is given by $T_X \sim t^{\nu}$.

For $T\xi \gg 1$ finite-size effects dominate, and we enter the 'quantum critical' region. $\Psi(x) \sim \mathcal{O}(1)$ as $x \to \infty$ so that $\chi \sim T^{-\frac{\gamma}{\nu}}$ in the quantum critical region.

In terms of RG flow, the free energy density at a particular point in parameter space is dominated by the singular behaviour of fixed point $F$ if the RG trajectory that starts there spends a long 'RG time' in the vicinity of the point $F$. Because RG flow is slow in the vicinity of the fixed point, it suffices for the trajectory to pass close to the fixed point. The trajectories in the classical region all pass close to the $F_d$ fixed point, which means that the free energy here is dominated by the singular behaviour associated with $F_d$ critical exponents.

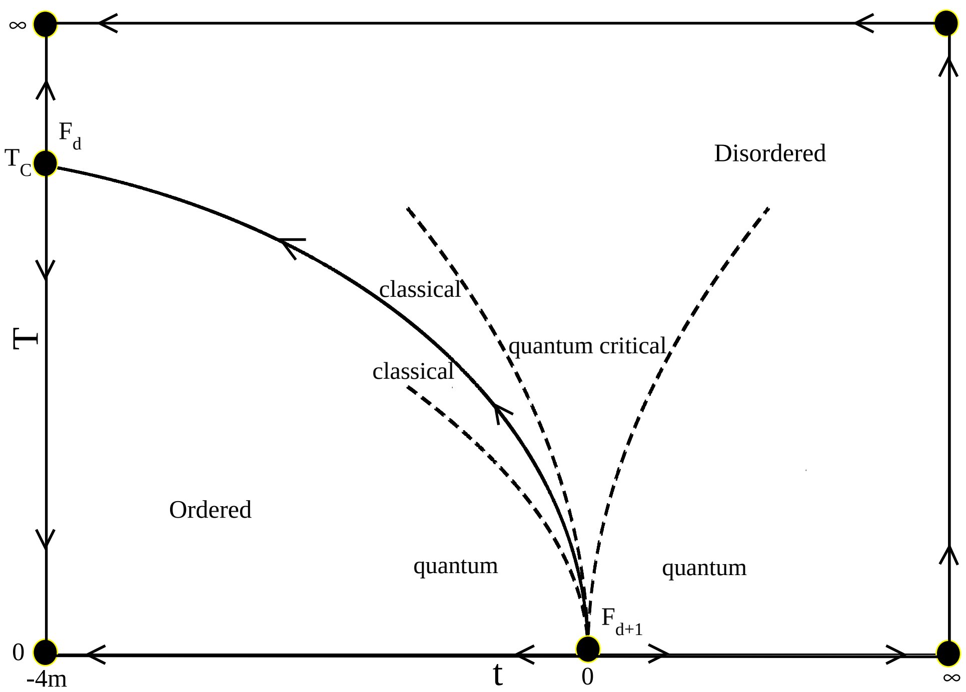


Figure 6.4: RG flow around the quantum critical point. Understanding quantum critical behaviour is one of the finest applications of RG scaling.