

# Advanced Quantum Theory

**Lecturer:** Sebastian Müller (HH 4.08, [sebastian.muller@bristol.ac.uk](mailto:sebastian.muller@bristol.ac.uk))

**Lectures:** Mon 2-4pm (TCC room) for 8 weeks

**Problem classes:** Wed 12 noon (SM4)  
(in some weeks starting 1 Feb, not transmitted)

**Drop in session:** Thu 10:30-11:30, Fri 10:30-11:30

**Course page:** [sebastianmueller.weebly.com/aqt.html](http://sebastianmueller.weebly.com/aqt.html)

**weekly problem sheets** (starting next week)

**for MSci/MSc students:** assessment by exam

**for PhD students:** assessment by homework  
can be emailed from outside Bristol

also email [graduate.studies@maths.ox.ac.uk](mailto:graduate.studies@maths.ox.ac.uk) to register

# Syllabus

- basics
- Feynman path integral
- perturbation theory
- second quantisation
- connection between path integral + second quantisation

## Books

- Condensed matter field theory (Altland, Simons)
- Quantum field theory for the gifted amateur (Lancaster, Blundell)
- Path integral methods in quantum field theory (Rivers)
- Path Integral Methods and Applications (outline notes by R. MacKenzie, <http://arxiv.org/pdf/quant-ph/0004090v1.pdf>)

more references in unit description

# 1 Basics

## 1.1 Classical mechanics

### Lagrange

$$q = (q_1, q_2, \dots)$$

$$L(q, \dot{q}, t) = T - U$$

$$\boxed{\frac{\partial L}{\partial q_\alpha} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\alpha}} \Leftrightarrow \text{action } S[q] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t) dt \text{ is stationary}^{t_1}$$

### Hamilton

use  $q_\alpha$  and  $p_\alpha = \frac{\partial L}{\partial \dot{q}_\alpha}$  as variables

$$H(q, p, t) = p \cdot \dot{q} - L$$

$$\boxed{\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha}, \quad \dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha}}$$

## 1.2 Quantum mechanics

$$q_\alpha \rightarrow Q_\alpha = \hat{q}_\alpha$$

$$p_\alpha \rightarrow P_\alpha = \hat{p}_\alpha = \frac{\hbar}{i} \frac{\partial}{\partial q_\alpha}$$

$$\boxed{\hat{H} \psi(q, t) = i\hbar \frac{\partial}{\partial t} \psi(q, t)}$$

write  $\uparrow_{\underline{r}}$  from now on

bra-ket / Dirac notation

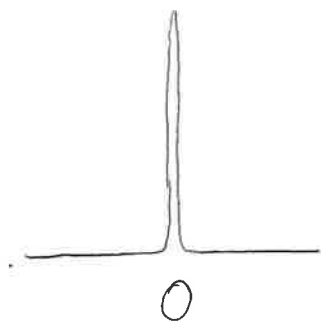
$$\psi(\underline{r}) \rightarrow |\psi\rangle$$

scalar product

$$\int \varphi^*(\underline{r}) \psi(\underline{r}) d^n r = \langle \varphi | \psi \rangle$$

for eigenfunctions one often writes the eigenvalue inside the bracket

# Delta function $\delta(\underline{r})$



informal definition:

$$\delta(\underline{r}) = 0 \text{ for } \underline{r} \neq 0$$

$\delta(\underline{r})$  diverges at  $\underline{r} = 0$

$$\int f(\underline{r}) \delta(\underline{r}) d^n r = f(0)$$

QM interpretation:

$\delta(\underline{r})$  is wavefunction of particle localised at  $\underline{r} = 0$

i.e. position eigenfunction with eigenval 0,  $|0\rangle$

$\delta(\underline{r} - \underline{r}')$  is wavefunction of particle localised at  $\underline{r} = \underline{r}'$

i.e. position eigenfunction with eigenval  $\underline{r}'$ ,  $|\underline{r}'\rangle$

use of  $\langle \underline{r}' |$  :

$$\langle \underline{r}' | \psi \rangle = \int \delta(\underline{r} - \underline{r}') \psi(\underline{r}) d^n r = \psi(\underline{r}')$$

integral representation:

$$\frac{1}{(2\pi\hbar)^n} \int e^{\frac{i}{\hbar} \underline{p} \cdot \underline{r}} d^n p = \delta(\underline{r})$$

# Resolution of the identity

for discrete basis:

$$\sum_m |m\rangle \langle m| = \mathbb{1}$$

for position eigenfunctions:

$$\int |\underline{r}\rangle \langle \underline{r}| d^n r = \mathbb{1}$$

Proof:

$$\begin{aligned} & \langle \varphi | \int |\underline{r}\rangle \langle \underline{r}| d^n r | \psi \rangle \\ &= \int \langle \varphi | \underline{r} \rangle \langle \underline{r} | \psi \rangle d^n r \\ & \quad \underbrace{\hspace{1.5cm}}_{= \langle \underline{r} | \varphi \rangle^*} \quad \underbrace{\hspace{1.5cm}}_{\psi(\underline{r})} \\ & \quad = \varphi(\underline{r})^* \psi(\underline{r}) \\ &= \langle \varphi | \psi \rangle \\ &= \langle \varphi | \mathbb{1} | \psi \rangle \quad \text{for all } \varphi, \psi \end{aligned}$$

# Time evolution

Schrödinger equation solved by

$$\psi(\mathbf{r}, t) = e^{-\frac{i}{\hbar} \hat{H} t} \psi(\mathbf{r}, 0)$$

time ↑ evolution operator

$$e^{-\frac{i}{\hbar} \hat{H} t} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \hat{H} t\right)^n$$

Propagator:

$$K(\mathbf{r}_f, \mathbf{r}_0, t) = \langle \mathbf{r}_f | e^{-\frac{i}{\hbar} \hat{H} t} | \mathbf{r}_0 \rangle$$

consider  
wavefunction  
at  $\mathbf{r}_f$

for  $t=0$  state localised at  $\mathbf{r}_0$

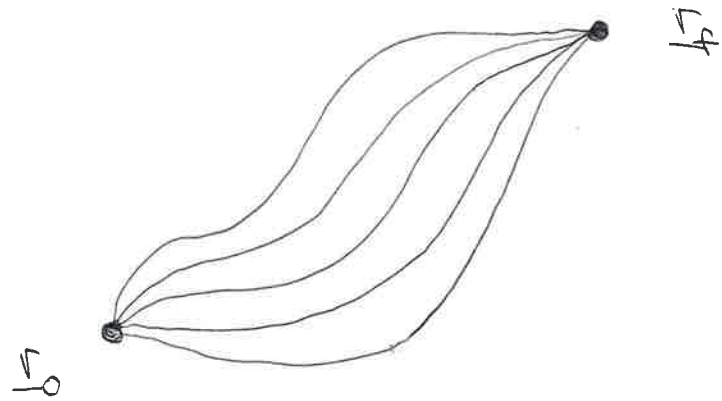
for  $t>0$  this state is evolved over time  $t$



## 2 Feynman path integral

$$K(\underline{r}_f, \underline{r}_0, t) = \int \mathcal{D}[\underline{r}] e^{\frac{i}{\hbar} S[\underline{r}]}$$

integral over all  $\int$  paths that go from  $\underline{r}_0$  to  $\underline{r}_f$  in time  $t$



paths are given by functions  $\underline{r}(t')$  with  $\underline{r}(0) = \underline{r}_0$   
 $\underline{r}(t) = \underline{r}_f$

## 2.1 Short times

consider  $\hat{H} = \underbrace{\frac{\hat{p}^2}{2m}}_{\hat{T}} + \hat{U}(\hat{r})$

$$K(r_f, r_0, t) = \langle r_f | e^{-\frac{i}{\hbar}(\hat{T} + \hat{U})t} | r_0 \rangle$$

would like  
 $e^{-\frac{i}{\hbar}\hat{T}t} e^{-\frac{i}{\hbar}\hat{U}t}$

$$\simeq \langle r_f | (1 - \frac{i}{\hbar}(\hat{T} + \hat{U})t) | r_0 \rangle$$

↑  
for small  $t$  (linear order)

$$\simeq \langle r_f | (1 - \frac{i}{\hbar}\hat{T}t)(1 - \frac{i}{\hbar}\hat{U}t) | r_0 \rangle$$

$$\simeq \langle r_f | e^{-\frac{i}{\hbar}\hat{T}t} \underbrace{e^{-\frac{i}{\hbar}\hat{U}t}}_{= e^{-\frac{i}{\hbar}U(r_0)t} | r_0 \rangle} | r_0 \rangle$$

$$= \underbrace{\langle r_f | e^{-\frac{i}{\hbar}\hat{T}t} | r_0 \rangle}_{=: A} e^{-\frac{i}{\hbar}U(r_0)t}$$

## Evaluation of A:

$$\begin{aligned} A &= \int \delta(\underline{r} - \underline{r}_f) e^{-\frac{i}{\hbar} \hat{T} t} \delta(\underline{r} - \underline{r}_0) d^n r \\ &= \int \delta(\underline{r} - \underline{r}_f) e^{-\frac{i}{\hbar} \hat{T} t} \left( \frac{1}{(2\pi\hbar)^n} \int e^{\frac{i}{\hbar} \underline{p} \cdot (\underline{r} - \underline{r}_0)} d^n p \right) d^n r \\ &= \frac{1}{(2\pi\hbar)^n} \int d^n r \delta(\underline{r} - \underline{r}_f) \int d^n p e^{-\frac{i}{\hbar} \hat{T} t} e^{\frac{i}{\hbar} \underline{p} \cdot (\underline{r} - \underline{r}_0)} \end{aligned}$$

Now use

$$\begin{aligned} \hat{p} e^{\frac{i}{\hbar} \underline{p} \cdot (\underline{r} - \underline{r}_0)} &= \frac{\hbar}{i} \frac{\partial}{\partial \underline{r}} e^{\frac{i}{\hbar} \underline{p} \cdot (\underline{r} - \underline{r}_0)} \\ &= \frac{\hbar}{i} \frac{i}{\hbar} \underline{p} e^{\frac{i}{\hbar} \underline{p} \cdot (\underline{r} - \underline{r}_0)} \end{aligned}$$

↳ analogous result holds for all powers + functions of  $\hat{p}$

$$\begin{aligned} &= \frac{1}{(2\pi\hbar)^n} \int d^n r \delta(\underline{r} - \underline{r}_f) \int d^n p e^{-\frac{i}{\hbar} \frac{\underline{p}^2}{2m} t} e^{\frac{i}{\hbar} \underline{p} \cdot (\underline{r} - \underline{r}_0)} \\ &= \frac{1}{(2\pi\hbar)^n} \int d^n p e^{-\frac{i}{\hbar} \frac{\underline{p}^2}{2m} t + \frac{i}{\hbar} \underline{p} \cdot (\underline{r}_f - \underline{r}_0)} \\ &= \prod_{k=1}^n \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp_k e^{-\frac{i}{\hbar} \frac{p_k^2}{2m} t + \frac{i}{\hbar} p_k (r_{fk} - r_{0k})} \end{aligned}$$

## Integrals:

Gauss:  $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$

Fresnel:  $\int_{-\infty}^{\infty} e^{+iax^2} dx = \sqrt{\frac{\pi}{+ia}} \left( = \sqrt{\frac{\pi}{|a|}} e^{+i\frac{\pi}{4} \text{sgn} a} \right)$

## shifted Fresnel:

$$\begin{aligned} & \int_{-\infty}^{\infty} \exp(-iax^2 + ibx) dx \\ &= \int_{-\infty}^{\infty} \exp\left(-ia\left(x - \frac{b}{2a}\right)^2 + ia\frac{b^2}{4a^2}\right) dx \\ & \stackrel{y = x - \frac{b}{2a}}{=} \int_{-\infty}^{\infty} \exp(-ia y^2) dy \exp\left(i\frac{b^2}{4a}\right) \\ & \quad \underbrace{\hspace{10em}} \\ & \quad = \sqrt{\frac{\pi}{ia}} \end{aligned}$$

use this for the factors in

$$A = \prod_{k=1}^n \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp_k \exp\left(-\frac{i}{\hbar} \frac{p_k^2}{2m} t + \frac{i}{\hbar} p_k (r_{fk} - r_{ok})\right)$$

(with  $a = \frac{t}{2m\hbar}$ ,  $b = \frac{r_{fk} - r_{ok}}{\hbar}$ )

$$A = \prod_{k=1}^n \left(\frac{m}{2\pi i \hbar t}\right)^{1/2} \exp\left(\frac{i}{\hbar} \frac{1}{2} m \left(\frac{r_{fk} - r_{ok}}{t}\right)^2 t\right)$$

## Propagator

$$K(r_f, r_0, t) \approx \left(\frac{m}{2\pi i \hbar t}\right)^{n/2} \exp\left(\frac{i}{\hbar} \left[ \frac{1}{2} m \left(\frac{r_f - r_0}{t}\right)^2 - U(r_0) \right] t\right)$$

for small  $t$ ,  
 $r_f$  close to  $r_0$

good appr. for  
kin. energy  
on trajectory

good appr.  
for pot.  
energy

good approx. for L

good approx. for S

## 2.2 Arbitrary times

divide  $t$  into intervals of size  $\tau = \frac{t}{N}$ ,  $N \rightarrow \infty$

$$K(\underline{r}_f, \underline{r}_0, t) = \langle \underline{r}_f | e^{-\frac{i}{\hbar} \hat{H} \tau} e^{-\frac{i}{\hbar} \hat{H} \tau} \dots e^{-\frac{i}{\hbar} \hat{H} \tau} | \underline{r}_0 \rangle$$

$$\mathbb{1} = \int d^n r_{N-1} | \underline{r}_{N-1} \rangle \langle \underline{r}_{N-1} | \quad \mathbb{1} = \int d^n r_1 | \underline{r}_1 \rangle \langle \underline{r}_1 |$$

$$= \int d^n r_1 \dots d^n r_{N-1} \langle \underline{r}_f | e^{-\frac{i}{\hbar} \hat{H} \tau} | \underline{r}_{N-1} \rangle \langle \underline{r}_{N-1} | e^{-\frac{i}{\hbar} \hat{H} \tau} | \underline{r}_{N-2} \rangle \dots \langle \underline{r}_1 | e^{-\frac{i}{\hbar} \hat{H} \tau} | \underline{r}_0 \rangle$$

↑  
set  $\underline{r}_N := \underline{r}_f$

$$= \int d^n r_1 \dots d^n r_{N-1} \prod_{j=0}^{N-1} \langle \underline{r}_{j+1} | e^{-\frac{i}{\hbar} \hat{H} \tau} | \underline{r}_j \rangle$$

$$\approx \left( \frac{m}{2\pi i \hbar \tau} \right)^{n/2} \exp\left( \frac{i}{\hbar} \left[ \frac{1}{2} m \left( \frac{\underline{r}_{j+1} - \underline{r}_j}{\tau} \right)^2 - \mathcal{U}(\underline{r}_j) \right] \tau \right)$$

$$\approx \left( \frac{m N}{2\pi i \hbar t} \right)^{nN/2} \int d^n r_1 \dots d^n r_{N-1} \exp\left( \frac{i}{\hbar} \sum_{j=0}^{N-1} \left[ \frac{1}{2} m \left( \frac{\underline{r}_{j+1} - \underline{r}_j}{\tau} \right)^2 - \mathcal{U}(\underline{r}_j) \right] \tau \right)$$