Advanced Quantum Theory

Lecturer: Sebastian Müller (HH 4.08, 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

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 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 (online notes by R. MacKenzie, http://arxiv.org/pdf/quant-ph/0004090v1.pdf)

more references in unit description

1 Basics

1.1 Classical mechanics

Lagrange

$\underline{q} = (q_1, q_2, \dots)$

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

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

Hamilton

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

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

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

1.2 Quantum mechanics

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

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

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

write $\underline{r}$ from now on

bra-ket / Dirac notation

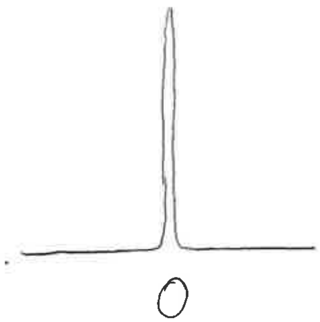
$$\psi(\underline{r}) \longrightarrow |\psi\rangle$$

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:

$\delta(\underline{r}) = 0$ 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:

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

for **position eigenfunctions**:

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

Proof:

$$\langle\varphi| \int |\underline{r}\rangle\langle\underline{r}|\, d^n r\, |\psi\rangle$$

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

$$= \langle\varphi|\psi\rangle$$

$$= \langle\varphi|\mathbb{1}|\psi\rangle \quad \text{for all } \varphi, \psi$$

Time evolution

Schrödinger equation solved by

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

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:

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

Consider wave function at $\underline{r}_f$

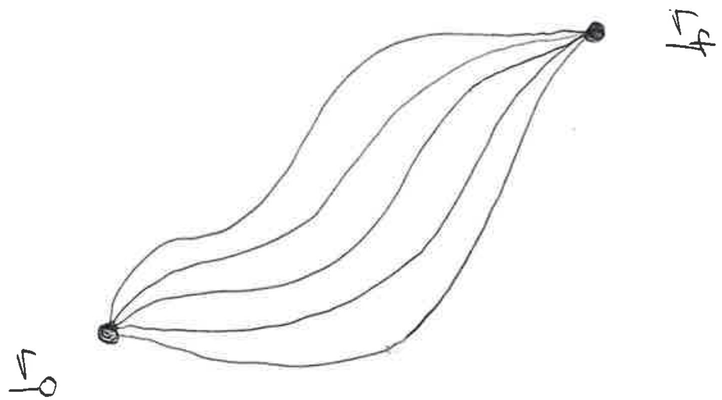
for $t=0$ state localised at $\underline{r}_0$

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

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 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
$e^{-\frac{i}{\hbar}\hat{T}t} e^{-\frac{i}{\hbar}\hat{u}t}$

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

for small t (linear order)

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

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

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

Evaluation of A:

$$A = \int \delta(\underline{r}-\underline{r}_f)\, e^{-\frac{i}{\hbar}\hat{T}t}\, \delta(\underline{r}-\underline{r}_0)\, d^n r$$

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

$$= \frac{1}{(2\pi\hbar)^n} \int d^n r\, \delta(\underline{r}-\underline{r}_f) \int d^n p\, e^{-\frac{i}{\hbar}\hat{T}t}\, e^{\frac{i}{\hbar}\underline{p}\cdot(\underline{r}-\underline{r}_0)}$$

now use

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

$$= \cancel{\frac{\hbar}{i}\frac{i}{\hbar}}\, \underline{p}\, e^{\frac{i}{\hbar}\underline{p}\cdot(\underline{r}-\underline{r}_0)}$$

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

$$= \frac{1}{(2\pi\hbar)^n} \int d^n r\, \delta(\underline{r}-\underline{r}_f) \int d^n p\, e^{-\frac{i}{\hbar}\frac{\underline{p}^2}{2m}t}\, e^{\frac{i}{\hbar}\underline{p}\cdot(\underline{r}-\underline{r}_0)}$$

$$= \frac{1}{(2\pi\hbar)^n} \int d^n p\, e^{-\frac{i}{\hbar}\frac{\underline{p}^2}{2m}t + \frac{i}{\hbar}\underline{p}\cdot(\underline{r}_f-\underline{r}_0)}$$

$$= \prod_{k=1}^{n} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp_k\, e^{-\frac{i}{\hbar}\frac{p_k^2}{2m}t + \frac{i}{\hbar}p_k(r_{fk}-r_{0k})}$$

Integrals:

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

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

shifted Fresnel:

$$\int_{-\infty}^{\infty} \exp(-iax^2 + ibx)\,dx$$

$$= \int_{-\infty}^{\infty} \exp\left(-ia\left(x - \frac{b}{2a}\right)^2 + ia\frac{b^2}{4a^2}\right) dx$$

$$\underset{y = x - \frac{b}{2a}}{=} \underbrace{\int_{-\infty}^{\infty} \exp(-iay^2)\,dy}_{= \sqrt{\frac{\pi}{ia}}}\ \exp\left(i\frac{b^2}{4a}\right)$$

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

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

Propagator

$$K(\underline{r}_f, \underline{r}_o, t) \simeq \left(\frac{m}{2\pi i\hbar t}\right)^{n/2} \exp\left(\frac{i}{\hbar}\underbrace{\underbrace{\left[\underbrace{\frac{1}{2}m\left(\frac{\underline{r}_f - \underline{r}_o}{t}\right)^2}_{\text{good appr. for kin. energy on trajectory}} - \underbrace{U(\underline{r}_o)}_{\text{good appr. for pot. energy}}\right]}_{\text{good approx. for } L} t}_{\text{good approx. for } S}\right)$$

for small t,
$\underline{r}_f$ close to $\underline{r}_o$

2.2 Arbitrary times

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

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

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

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

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

$$= \int d^n r_1 \dots d^n r_{N-1} \prod_{j=0}^{N-1} \underbrace{\langle \underline{r}_{j+1} | e^{-\frac{i}{\hbar}\hat{H}\tau} | \underline{r}_j \rangle}_{\simeq \left(\frac{m}{2\pi i \hbar \tau}\right)^{n/2} \exp\left(\frac{i}{\hbar}\left[\frac{1}{2} m \left(\frac{\underline{r}_{j+1} - \underline{r}_j}{\tau}\right)^2 - \mathcal{U}(\underline{r}_j)\right]\tau\right)}$$

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