Quantum Mechanics II

lecture notes

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Notes
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Contents

Introduction

These are my lecture notes of the lecture. You are welcome to tell any mistakes to: mmaetz AT student.ethz.ch. Unfortunately, some lectures are missing because lenovo/IBM is incompetent to give me a working laptop (thinkpad) after two months (even after about 30 e-mails and 10 phone calls).

Missing lectures

- 9th April
- 23th Mai

Chapter 1

Approximation methods for stationary problems

- standard QM problem:
  - given $|\psi(t_0)\rangle$
  - wanted

$$
\begin{aligned}
|\psi(t)\rangle &= U\left(t, t_0\right)|\psi(t_0)\rangle \\
U &= e^{-\frac{i}{\hbar}H(t-t_0)}
\end{aligned}
$$

- for time independent H

$$U = e^{-\frac{i}{\hbar}H(t-t_0)} \tag{1.1}$$

find eigenvalue and eigenstates (diagonalize H)

but: most problems cannot be solved exactly → find approximate solution.

1.1 Time-independent perturbation theory, non-degenerate case

Assume:

$$H = H_0 + \lambda V \tag{1.2}$$

with H_0 the Hamiltonian that I can solve ("free" Hamiltonian) and the perturbation V "small" and λ a dimensionless bookkeeping part.

$$
\begin{aligned}
&\lambda \to 0, \quad H \to H_0 \\
&\lambda \to 1, \quad \text{full } H
\end{aligned}
$$

We know

$$\left|\psi_n^{(0)}\right\rangle, E_n^{(0)}$$

with

$$H_0\left|\psi_n^{(0)}\right\rangle = E_n^{(0)}\left|\psi_n^{(0)}\right\rangle$$

with

$$\left\langle\psi_n^{(0)}\middle|\psi_m^{(0)}\right\rangle = \delta_{mn}$$

(continuous spectrum also understood.)
We want $|\psi_n\rangle$ and E_n with

$$(H_0 + \lambda V)\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

let

$$\begin{aligned} E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \\ \left|\psi_n\right\rangle &= \left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + \dots \end{aligned}$$

seems obvious, but assumption. (convergence?)

$$\begin{aligned} &\left(H_0 - E_n^{(0)}\right)\left|\psi_n^{(0)}\right\rangle + \lambda\left(\left(H_0 - E_n^{(0)}\right)\left|\psi_n^{(1)}\right\rangle\right) \\ &\quad + \lambda^2\left(\left(H_0 - E_n^{(0)}\right)\left|\psi_n^{(2)}\right\rangle + \left(V - E_n^{(1)}\right)\left|\psi_n^{(1)}\right\rangle - E_n^{(2)}\right) + \mathcal{O}\left(\lambda^3\right) = 0 \end{aligned}$$

with $\mathcal{O}(1)$ "step 0", $\mathcal{O}(\lambda)$ "step 1", $\mathcal{O}(\lambda^2)$ "step 2".

Step 0: nothing to do

Step 1 multiply by $\left\langle\psi_m^{(0)}\right|$

$$\begin{aligned} &\left\langle\psi_m^{(0)}\right| H_0 - E_n^{(0)}\left|\psi_m^{(0)}\right\rangle + \left\langle\psi_m^{(0)}\right| V - E_n^{(1)}\left|\psi_m^{(0)}\right\rangle = 0 \\ &= \left(E_m^{(0)} - E_n^{(0)}\right)\left\langle\psi_m^{(0)}\middle|\psi_n^{(1)}\right\rangle + \left\langle\psi_m^{(0)}\right| V\left|\psi_m^{(0)}\right\rangle - E_n^{(1)}\delta_{mn} = 0 \end{aligned}$$

to get $\left|\psi_n^{(1)}\right\rangle$

$$\begin{aligned} \left|\psi_n^{(1)}\right\rangle &= \sum_m \underbrace{\left\langle\psi_m^{(0)}\middle|\psi_n^{(1)}\right\rangle}\left|\psi_m^{(0)}\right\rangle \\ &= \sum_m \frac{\left\langle\psi_m^{(0)}\right| V\left|\psi_m^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}}\left|\psi_m^{(0)}\right\rangle + \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\middle|\psi_n^{(1)}\right\rangle \end{aligned}$$

from normalization

$$\langle \psi_n | \psi_n \rangle \stackrel{!}{=} 1 = \underbrace{\left\langle \psi_n^{(0)} \middle| \psi_n^{(0)} \right\rangle}_{1} + \lambda \underbrace{\left\langle \psi_n^{(0)} \middle| \psi_n^{(1)} \right\rangle}_{0} + \lambda \left\langle \psi_n^{(1)} \middle| \psi_n^{(0)} \right\rangle + \mathcal{O}\left(\lambda^2\right) \quad (1.3)$$

has to be small. If $E_n^{(0)} = E_m^{(0)}$?? degeneracy! $\rightarrow$ sec 1.2 if $E_n^{(0)} \simeq E_m^{(0)}$ quasi degenerate

step 2 take $\mathcal{O}(\lambda^2)$ terms $\left\langle \psi_k^{(0)} \right|$

$$\left(E_k^{(0)} - E_n^{(0)}\right) \left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle + \left\langle \psi_k^{(0)} \middle| V \middle| \psi_k^{(0)} \right\rangle - E_n^{(1)} \left\langle \psi_k^{(0)} \middle| \psi_n^{(1)} \right\rangle = E_n^{(2)} \delta_{kn} \quad (1.4)$$

for $k = n$

$$\begin{aligned} E_n^{(2)} &= \left\langle \psi_n^{(0)} \middle| V \middle| \psi_n^{(0)} \right\rangle \\ &= \sum_{m \neq n} \frac{\left\langle \psi_n^{(0)} \middle| V \middle| \psi_n^{(0)} \right\rangle \left\langle \psi_m^{(0)} \middle| V \middle| \psi_m^{(0)} \right\rangle}{E_n^{(0)} - E_m^{(0)}} \\ &= \sum_{m \neq n} \frac{\left\| V_{nm}^2 \right\|}{E_n^{(0)} - E_m^{(0)}} \end{aligned} \quad (1.5)$$

Note $E_n^{(2)} < 0$ for ground state.
Next compute $\left| \psi_n^{(2)} \right\rangle$: initially fix normalization such that

$$\left\langle \psi_n^{(0)} \middle| \psi_n^{(i)} \right\rangle = \delta_{i0} \quad (1.6)$$

this is in conflict

$$\langle \psi_n | \psi_n \rangle = 1 \quad (1.7)$$

$\rightarrow$ sort out at the end.

$$\begin{aligned} \left| \psi_n^{(2)} \right\rangle &= \sum_{k \neq n} \left| \psi_k^{(0)} \right\rangle \left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle + 0 \\ &= \sum_{k \neq n} \left| \psi_k^{(0)} \right\rangle \left(\frac{\left\langle \psi_k^{(0)} \middle| V \middle| \psi_k^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} - \frac{E_n^{(1)} \left\langle \psi_k^{(0)} \middle| \psi_n^{(1)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} \right) \end{aligned} \quad (1.8)$$

plug in $\left|\psi_n^{(1)}\right\rangle$ and sort out normalization

$$|\psi_n\rangle_N = \mathbb{Z}^{1/2}\,|\psi_n\rangle \tag{1.9}$$

fix such that

$$_N\,\langle\psi_n|\psi_n\rangle_M = 1 \tag{1.10}$$

$$\begin{aligned}
_N\,\langle\psi_n|\psi_n\rangle_N &= 1\\
&= Z_n\,\langle\psi_n|\psi_n\rangle\\
&= Z_n\left(\left\langle\psi_n^{(0)}\right| + \lambda\left\langle\psi_n^{(1)}\right| + \lambda^2\left\langle\psi_n^{(2)}\right|\right)\\
&\quad\times\left(\left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \dots\right)\\
&= E_n^{(2)}\delta_{kn}\\
&= Z_n\left(1 + \lambda^2\left\langle\psi_n^{(1)}\middle|\psi_n^{(1)}\right\rangle + \mathcal{O}\left(\lambda^3\right)\right)
\end{aligned} \tag{1.11}$$

$$Z_n^{1/2} = 1 - \frac{\lambda^2}{2}\left\langle\psi_n^{(1)}\middle|\psi_n^{(1)}\right\rangle\mathcal{O}\left(\lambda^3\right) \tag{1.12}$$

$$\begin{aligned}
&\Rightarrow \left|\psi_n^{(2)}\right\rangle\\
&= \sum_{k\neq n}\sum_{m\neq n}\left|\psi_k^{(0)}\right\rangle\left[\frac{V_{km} - V_{mn}}{\left(E_n^{(0)} - E_k^{(0)}\right)\left(E_m^{(0)} - E_n^{(0)}\right)} - \frac{V_{kn}V_{nn}}{\left(E_n^{(0)} - E_n^{(0)}\right)}\right]\\
&\quad - \frac{1}{2}\sum_{k\neq n}\left|\psi_n^{(0)}\right\rangle\frac{\left\|V_{kn}^2\right\|}{\left(E_n^{(0)} - E_k^{(0)}\right)}
\end{aligned} \tag{1.13}$$

1.2 Time-independent perturbation theory: degenerate case

Assume $E_n^{(0)}$ is α-fold degenerate i.e.

$$H_0\left|\psi_{n_i}^{(0)}\right\rangle = E_n^{(0)}\left|\psi_n^{(0)}\right\rangle, \quad 1 \leq i \leq \alpha \tag{1.14}$$

fix

$$\left\langle\psi_{n_i}^{(0)}\middle|\psi_{n_j}^{(0)}\right\rangle = \delta_{ij} \tag{1.15}$$

Any linear combination

$$\left|\chi_n^{(0)}\right\rangle = \sum_{i=1}^{\alpha} c_{n_i}\left|\psi_{n_i}^{(0)}\right\rangle \tag{1.16}$$

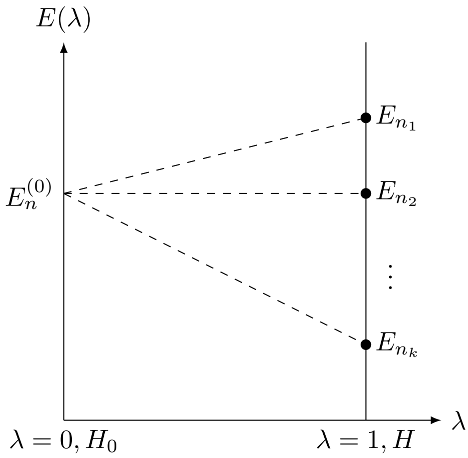

Figure 1.1:

is an eigenstate of H_0 with evaluation $E_n^{(0)}$ Typically V "lifts" degeneracy at least partially since often

$$[H_0, V] \neq 0 \tag{1.17}$$

Pick one of the evals E_{n_k} with

$$H\left|\psi_{n_k}\right\rangle = E_{n_k}\left|\psi_{n_k}\right\rangle \tag{1.18}$$

for $\lambda \to 0$: $E_{n_k} \to E_n^{(0)}$ and

$$\begin{aligned}\left|\psi_{n_k}\right\rangle &\to \left|\chi_{n_k}(0)\right\rangle \\ &= \sum_{i=1}^{\alpha} \underbrace{c_{n_k i}\left|\psi_{n_i}^{(0)}\right\rangle}_{\substack{\text{some lin}\\ \text{comb}}}\end{aligned} \tag{1.19}$$

have to find "good" linear combination, i.e. coeff $c_{n_k i}$. Main idea as before:

$$\left|\psi_{n_k}\right\rangle = \left|\chi_{n_k}^{(0)}\right\rangle + \lambda\left|\psi_{n_k}^{(1)}\right\rangle \tag{1.20}$$

$$0 = \left(H_0 - E_n^{(0)}\right)\left|\psi_{n_k}^{(1)}\right\rangle + \left(V - E_{n_k}^{(1)}\right)\left|\chi_{n_k}^{(1)}\right\rangle \tag{1.21}$$

with

$$\left|\psi_{n_k}^{(1)}\right\rangle = \sum_{\ell=1}^{\dim(H_0)} a_{n_\ell}\left|\psi_{\ell}^{(0)}\right\rangle \tag{1.22}$$

and

$$\sum_{i=1}^{\alpha} c_{n_k i} \left|\psi_{n_i}^{(0)}\right\rangle \tag{1.23}$$

multiply by $\left\langle\psi_{n_j}^{(0)}\right|$.

$$\sum_{\ell=1}^{\dim H_0} \underbrace{\left(E_\ell^{(0)} - E_n^{(0)}\right)}_{=0 \text{ for } n=\ell} a_{n\ell} \underbrace{\left\langle\psi_{n_j}^{(0)}\middle|\psi_\ell^{(0)}\right\rangle}_{=0 \text{ for } n\neq\ell} + \sum_{i=1}^{\alpha} c_{n_k i} \left(\left\langle\psi_{n_j}^{(0)}\right| V \left|\psi_{n_j}^{(0)}\right\rangle \right. \tag{1.24}$$
$$\left. - E_{n_k}^{(1)} \underbrace{\left\langle\psi_{n_j}^{(0)}\middle|\psi_{n_i}^{(0)}\right\rangle}_{V_{ji}} - E_{n_k}^{(1)} \underbrace{\left\langle\psi_{n_j}^{(0)}\middle|\psi_{n_i}^{(0)}\right\rangle}_{\delta_{ij}} \right)$$

$\rightarrow$ solve

$$\det \begin{pmatrix} V_{11} - E_{n_k}^{(1)} & V_{12} & \dots & V_{1\alpha} \\ V_{21} & V_{22} - E_{n_k}^{(1)} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ V_{\alpha 1} & \dots & \dots & V_{\alpha\alpha} - E_{n_k}^{(1)} \end{pmatrix} = 0 \tag{1.25}$$

$\rightarrow$ eq. of order $\propto$ in $E_{n_k}^{(1)}$
$\rightarrow$ α solutions

1.2.1 easy way out (sometimes)

if $V_{ij} = 0$ for $i \neq j$ problem already solved
$\rightarrow$ α solutions are

$$E_{n_i}^{(1)} = \left\langle\psi_i^{(0)}\right| V \left|\psi_i^{(0)}\right\rangle \tag{1.26}$$

Note: if $\exists$ operator A with

$$[A, V] = 0 \tag{1.27a}$$

and

$$A \left|\psi_{n_i}^{(0)}\right\rangle = a_{n_i} \left|\psi_{n_i}^{(0)}\right\rangle, \tag{1.27b}$$

with

$$a_{n_i} \neq a_{n_k}, \quad \text{for } k \neq i \tag{1.27c}$$

then these $\left|\psi^{(0)}_{n_i}\right\rangle$ are "good" eigenstates

Proof:

$$\begin{aligned} \left\langle\psi^{(0)}_{n_i}\right| [A, V] \left|\psi^{(0)}_{n_i}\right\rangle &= 0 \\ &= \underbrace{(a_{n_i} - a_{n_k})}_{\neq 0} \underbrace{\left\langle\psi^{(0)}_{n_i}\right| V \left|\psi^{(0)}_{n_i}\right\rangle}_{V_{ik}} \end{aligned} \tag{1.28a}$$

$$\Rightarrow V_{ik} = 0 \tag{1.28b}$$

1.3 The variational principle

Useful to get good estimate of ground-state energy E_0 of complicated systems. Claim

$$E_0 \leq \frac{\langle\psi| H |\psi\rangle}{\langle\psi|\psi\rangle} = \langle\psi| H |\psi\rangle \tag{1.29}$$

if $|\psi\rangle$ normalized.

Proof: Let

$$|\psi\rangle = \sum c_n |\psi_n\rangle\,, \tag{1.30a}$$

with

$$H |\psi_n\rangle = E_n |\psi_n\rangle \tag{1.30b}$$

and

$$\langle\psi|\psi\rangle = 1 \tag{1.30c}$$

$$\Rightarrow \sum \|c_n\|^2 = 1 \tag{1.30d}$$

then

$$\begin{aligned} \langle\psi| H |\psi\rangle &= \sum_{m,n} c^*_m c_n \langle\psi_m| H |\psi_m\rangle = \sum_{m,n} c^*_m c_n E_n \underbrace{\langle\psi_m|\psi_n\rangle}_{\delta_{mn}} \\ &= \sum_n \|c_n\|^2 E_n \geq E_0 \sum_n \|c_n\|^2 = E_0 \end{aligned} \tag{1.30e}$$

Example 1.3.1 (Harmonic oscillator):

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{m}{2}\omega^2 x^2 \tag{1.31}$$

(of course we know $E_0 = \frac{\hbar}{2}\omega$). Let

$$\psi(x) = Ae^{-bx^2} \tag{1.32a}$$

since

$$\begin{aligned}\langle\psi|\,\psi\rangle \overset{!}{=} 1 &= \int \mathrm{d}x\ \|A\|^2\, e^{-2bx^2} \\ &= \|A\|^2\sqrt{\frac{\pi}{2b}}\end{aligned} \tag{1.32b}$$

compute

$$\begin{aligned}\langle\psi|\,H\,|\psi\rangle &= \|A\|^2\int \mathrm{d}x\, e^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{m}{2}\omega^2x^2\right)e^{-bx^2} \\ &= \dots \\ &= \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b} \\ &= \langle\psi|\,H\,|\psi\rangle \\ &\geq E_0\end{aligned} \tag{1.32c}$$

Minimize with respect to b

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}b}\langle\psi|\,H\,|\psi\rangle &= \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} \\ &= 0\end{aligned} \tag{1.33a}$$

$$b_{\text{min}} = \frac{m\omega}{2\hbar} \tag{1.33b}$$

$$\begin{aligned}E_0 &\leq \langle\psi|\,H\,|\psi\rangle_{\text{min}} \\ &= \frac{\hbar\omega}{2}\end{aligned} \tag{1.33c}$$

in this case we get E_0 exactly is a coincidence, since Ansatz=true wave function.

1.4 WKB approximation, semiclassical approximation

WKB for Wentzel, Kramers, Brillouin (see QMI Ch. 8.3.) useful for 1-dim problems with "smooth" popential. Schrödinger:

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}V(x)\right)\psi(x) = E\psi(x) \tag{1.34a}$$

if

$$V(x) \equiv V_0 \text{ const.} \tag{1.34b}$$

$$\psi(x) = e^{\pm\frac{i}{\hbar}\sqrt{2m(E-V_0)}x} \tag{1.34c}$$

if $V(x)$ is slowly varying. Ansatz

$$\psi(x) = e^{\frac{i}{\hbar}S(x)} \tag{1.34d}$$

Ansatz into Schrödinger:

$$\frac{-i\hbar}{2m}S'' + \frac{1}{2m}\left(S'\right)^2 + V(x) - E = 0 \tag{1.34e}$$

equivalent to but more complicated than Schrödinger. Note for

$$V(x) \equiv V_0$$

$$S = \pm\sqrt{2m\left(E - V_0\right)} \cdot x$$

and

$$S'' = 0$$

first term $\sim \hbar$ vanishes for

$$V(x) \equiv V_0, \quad \text{(classical limit)}\,,$$

Let

$$S(x) = S_0(x) + \hbar S_1(x) + \mathcal{O}(\hbar^2) \tag{1.35a}$$

plug in into differential equation for S

$$\frac{1}{2m}\left(S_0'\right)^2 + V(x) - E = 0 \tag{1.35b}$$

$$\begin{aligned}\Rightarrow S_0' &= \pm\sqrt{2m\left(E - V(x)\right)} \\ &\equiv \pm p(x)\end{aligned} \tag{1.35c}$$

$$S_0'S_1' - \frac{1}{2}S_0'' = 0 \tag{1.35d}$$

$$\Rightarrow S_1' = \frac{i}{2}\frac{S_0''}{S_0'} = \frac{i}{2}\frac{p'(x)}{p(x)} \tag{1.35e}$$

solve these differential equation

$$S_0 = \pm \int^x \mathrm{d}x'\, p(x') \tag{1.35f}$$

$$S_1 = \frac{i}{2} \ln p(x) \tag{1.35g}$$

$$\begin{aligned} \Rightarrow \psi(x) &= A e^{\frac{i}{\hbar}(S_0 + \hbar_1)} \\ &= \frac{A_+}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int \mathrm{d}x'\, p(x')} + \frac{A_-}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int \mathrm{d}x'\, p(x')} \end{aligned} \tag{1.35h}$$

Chapter 2

The hydrogen atom

2.1 Basics

Two body problem proton (1)-electron (2)

$$H = -\frac{\hbar^2}{2m_2}\boldsymbol{\nabla}_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V\left(\mathbf{r}_1 - \mathbf{r}_2\right) \tag{2.1}$$

new variables

$$R = \frac{m_2 r_1 + m_2 r_2}{m_1 + m_2} \tag{2.2}$$

$$r = r_1 - r_2 \tag{2.3}$$

$$M = m_1 + m_2 \tag{2.4}$$

$$m = \frac{m_1 m_2}{m_1 + m_2} \tag{2.5}$$

$$H = -\frac{\hbar^2}{2M} \tag{2.6}$$

2.2 Spin-orbit term

naive "derivation"

(1) Electron with spin → magnetic dipole moment

$$\boldsymbol{\mu} = \frac{e}{m}\frac{g}{2}\mathbf{s}\,, \tag{2.7}$$

$$\mu = \frac{e}{T}\pi r^2\,, \quad s = \frac{2\pi}{T} m r^2\,, \quad g \simeq \text{ (from Dirac)} \tag{2.8}$$

(2) Electron feeds magnetic field due to the proton

$$\mathbf{E} \sim \frac{e}{r3}\mathbf{r} \tag{2.9}$$

$$\begin{aligned} \rightarrow \mathbf{B} &= -\frac{1}{c^2}\boldsymbol{\nabla} \times \mathbf{E} \\ &= -\frac{1}{mc^2 r^3}\mathbf{p} \times \mathbf{r} \\ &= \frac{-\mathbf{L}}{mc^2 r^3} \end{aligned} \tag{2.10}$$

wrong by factor 2 (Thomas precession)

...correct result

$$H_{\text{SO}} = \frac{Ze^2}{2mc^2}\frac{1}{r^3}\mathbf{L}\cdot\mathbf{S}, \quad (\sim -\boldsymbol{\mu}\cdot\mathbf{B}) \tag{2.11}$$

To describe spin

$$\begin{aligned} \left| n, \ell, \left(s = \frac{1}{2}, m_s\right)\right\rangle &= \psi_{n\ell m_\ell m_s} \\ &= \psi_{n\ell m_\ell}(r, \theta\varphi)\,\chi_{m_s} \end{aligned} \tag{2.12a}$$

with χ_{m_s} spin-orbit

$$\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \tag{2.12b}$$

Note H_{SO} "mixes" states with same ℓ, but different m_ℓ, m_ℓ'
$\rightarrow$ use degenerate perturbation theory with $2\cdot(2\ell+1)\times\underbrace{2}_{\text{spin}}\underbrace{(2\ell+1)}_{m_\ell}$ matrix

$$\langle n, \ell, m_\ell', m_s'|\, H_{\text{SO}}\, |n, \ell, m_\ell', m_s'\rangle \rightarrow \text{diagonalize} \tag{2.13}$$

recall degenerate perturbation theory $\rightarrow$ find "good" linear combination that diagonalize this matrix by looking for symmetry use total angular momentum

$$J \equiv L + S \tag{2.14}$$

for $\ell = 0 \quad j = \frac{1}{2}$, for $\ell \neq 0 \quad j = \ell \pm \frac{1}{2}$. Use states

$$|n, \ell, j, m_j\rangle \tag{2.15}$$

$$|n,\ell,j,m_j\rangle = \sum_{m_\ell,m_s} |n,\ell,m_\ell,m_s\rangle \underbrace{\langle n,\ell,m_\ell,m_s|n,\ell,j,m_j\rangle}_{\text{Clebsch-Gordan}} \tag{2.16}$$

use

$$J^2 = L^2 + 2L\cdot S + S^2 \tag{2.17a}$$

$$L\cdot S = \frac{1}{2}\left(J^2 - L^2 - S^2\right) \tag{2.17b}$$

$|n,\ell,j,m_j\rangle$ are eigenstates of

$$H_0, L^2, S^2, J^2, J_z \tag{2.18}$$

with eigenvalues

$$E_n, \hbar^2\ell\left(\ell+1\right), \hbar^2\frac{3}{4}, \hbar^2 j\left(j+1\right), \hbar m_j \tag{2.19}$$

$$\Delta E_{\text{SO}} = \langle n,\ell,j,m_j|\, H_{\text{SO}}\, |n,\ell,j,m_j\rangle \tag{2.20}$$

for $\ell = 0$

$$\Delta E_{\text{SO}} = 0 \tag{2.21a}$$

for $\ell \neq 0$

$$\begin{aligned}
\Delta E_{\text{SO}} &= \frac{Ze^2}{2m^2c^2}\langle n,\ell,j,m_j|\,\frac{1}{r^3}\frac{1}{2}\left(J^2-L^2-S^2\right)|n,\ell,j,m_j\rangle \\
&= \frac{Ze^2}{2m^2c^2}\left\langle\frac{1}{r^3}\right\rangle\frac{\hbar^2}{2}\left(j\left(j+1\right)-\ell\left(\ell+1\right)-\frac{3}{4}\right) \\
&= -E_n\frac{\left(Z\alpha\right)^2}{2n\left(\ell+\frac{1}{2}\right)}\begin{cases}\frac{1}{\ell+1} & j=\ell+\frac{1}{2}\\ -\frac{1}{\ell} & j=\ell-\frac{1}{2}\end{cases}
\end{aligned} \tag{2.21b}$$

2.3 Darwin term

Sloppy consideration electron position fluctuates by $\delta r \simeq \lambda_c \simeq \frac{\hbar}{mc}$ electron feels average potential

$$\langle V\left(r+\delta r\right)\rangle = \langle V(r)\rangle + \underbrace{\frac{1}{2}\langle\boldsymbol{\delta}\rangle\, r\cdot\boldsymbol{\nabla}\boldsymbol{\delta} r\cdot\nabla V} \tag{2.22}$$

correct result is

$$\begin{aligned} H_D &= \frac{\hbar^2}{8m^2c^2}\nabla^2 V \\ &= \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\delta(r) \end{aligned} \tag{2.23}$$

only for $\ell = 0$!

$$\begin{aligned} \Delta E_D &= \langle n,\ell,j,m_j|\, H_D\, |n,\ell,j,m_j\rangle \\ &= \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\left\|\psi_{n\ell}(0)\right\|^2 \\ &= -E_n\frac{(Z\alpha)^2}{n}\delta_{\ell 0} \end{aligned} \tag{2.24}$$

2.4 Fine structure of hydrogen

Combine ΔE_{rel}, ΔE_{SO} and ΔE_D

$$\Delta E_n = -E_n^{(0)}\frac{(Z\alpha)^2}{n^2}\left(\frac{3}{4} - \frac{n}{j+\frac{1}{2}}\right) \tag{2.25}$$

valid for $\ell = 0$, i.e. $j = \frac{1}{2}$ and $j = \ell \pm \frac{1}{2}$.

fine structure suppressed $\sim (Z\alpha)^2$ relative to $E_n^{(0)}$ only depends on j (not independently on ℓ and s).

Notation for states nL_J

$$\begin{aligned} &n = 1, 2, \dots \\ &L \equiv S\,(\ell = 0)\,, P\,(\ell = 1)\,, D\,(\ell = 2)\,, F\,(\ell = 3) \end{aligned}$$

2.4.1 first few states

	$\ell = 0$	$\ell = 1$	$\ell = 2$	degeneracy $2n^2$
$n = 1$				

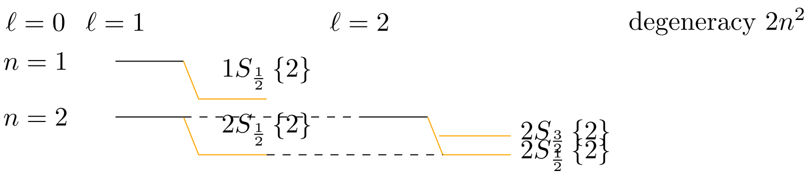

Figure 2.1:

2.5 Corrections beyound fine structure

2.5.1 Hyperfine structure

Effect of proton spin Sp

$$\boldsymbol{\mu}_p = \frac{e}{2m_p} g_p \mathbf{s}_p \tag{2.26}$$

μ_p indices B-field μ of electron "feels" B-field $\sim \boldsymbol{\mu} \cdot \mathbf{B}$

$$\rightsquigarrow \Delta E_{\text{Hfs}} \sim (Z\alpha)^4 \frac{m_e}{m_p}, \tag{2.27}$$

with $(Z\alpha)^4$ as always and $\frac{m_e}{m_p}$ suppression. total spin

$$\begin{aligned} F &= S_e + S_p \\ &= \begin{cases} 1 & \text{triplet} \\ 0 & \text{singlet} \end{cases} \end{aligned} \tag{2.28}$$

2.5.2 Lamb shift (needs QED!)

$\rightsquigarrow$ modification of Coulomb potential. splits e.g. $2S_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$

$$\Delta E_{\text{Lamb}} \sim (Z\alpha)^4 \cdot \alpha \left(\frac{1}{\log (Z\alpha)} \right) \dots \tag{2.29}$$

Chapter 3

Many Electron Atoms

$$H = \sum_{i=1}^{N} \left(\frac{p^2}{2m} - \frac{Ze^2}{r} \right) + \underbrace{\sum_{i>j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}}_{1} \tag{3.1}$$

$\rightarrow$ complicated! we want:

$$H\psi\left(1, \ldots, N\right) = E\psi\left(1, \ldots, N\right) \tag{3.2}$$

3.1 Identical particles

Consider N identical particles $H\left(1, .., N\right)$ wave function $\psi\left(1, \cdots, N\right)$.
In classical mechanics we can always distinguish these n particles state. In Quantum Mechanics, we cannot keep track of individual particles if their wave functions overlap. Defin permutation operator P_{ij} interchanging i and j

$$P_{ij}\psi\left(1, \ldots, i, \ldots, j, \ldots, N\right) = \psi\left(1, \ldots, j, \ldots, i, \ldots, N\right) \tag{3.3a}$$

$$P_{ij}^2 = 1 \tag{3.3b}$$

$$\Rightarrow \text{evals } \pm 1 \tag{3.3c}$$

[1]interaction between electrons

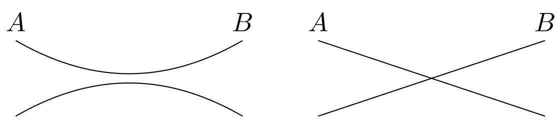

Figure 3.1:

H must be invariant under $i \leftrightarrow j$

$$\Rightarrow [H, P_{ij}] = 0 \tag{3.4}$$

There are $N!$ permutations of elements $1 \cdots N$, they fall into two classes, even and odd:

$$\mathrm{tr}(P) = \begin{cases} +1 & (-1)^2 \text{ even nr. of Interchanges} \\ -1 & (-1)^2 \text{ odd nr. of Interchanges} \end{cases} \tag{3.5}$$

we have $[H, P]$. P is unitary since

$$\begin{aligned} \langle \chi | \psi \rangle &= \langle P\xi | P\psi \rangle \qquad (3.6a) \\ &= \langle \xi | P^\dagger P |\psi\rangle \end{aligned}$$

$$\Rightarrow P^\dagger P = 1 \tag{3.6b}$$

for any observable A we have

$$[A, P] = 0\,. \tag{3.6c}$$

(*Identical* part) two combinations are important:

i) totally symmetric $|\psi\rangle_S$ with

$$P|\psi\rangle_S = |\psi\rangle_S \tag{3.7}$$

with $|\psi\rangle_S$ completely symmetric linear combination of all $N!$ Permutations.

ii) totalli antisymmetric $|\psi\rangle_A$ with

$$P|\psi\rangle_A = (-1)^P |\psi\rangle_A \tag{3.8}$$

...

3.2 Thomas-Fermi approximation

$\simeq$ semi classical: assume each electron feels average potential $\Phi(r)$, (spherically symmetric)

$$V = -\frac{Ze^2}{r} \xrightarrow{\text{other electron}} -e\Phi(r) \tag{3.9}$$

Poisson equation:

$$\boldsymbol{\nabla}^2 \Phi = -4\pi\tilde{\rho} \overset{r\geq 0}{=} 4\pi e \rho(r) \tag{3.10}$$

total charge density (other electron and nucleus)

$$\tilde{\rho} = -e\rho(r) + Ze\delta(r) \tag{3.11}$$

find relation between ρ and Φ. Let n be nr. states in certain energy range

$$n = \frac{2}{(2\pi\hbar)^3}, \quad \text{if } E = \frac{p^2}{2m} - e\Phi < 0 \tag{3.12a}$$

$$n = 0, \quad \text{if } E = \tfrac{p^2}{2m} - e\Phi > 0 \tag{3.12b}$$

$$\begin{aligned} \rho &= \int_0^{\sqrt{2me\Phi}} \mathrm{d}^3 p n \\ &= \frac{(4\pi)\, 2}{(2\pi\hbar)^3} \int_0^{\sqrt{2me\phi}} \end{aligned} \tag{3.12c}$$

plug this into Poisson $\to$ differential equation for Φ

$$\begin{aligned} \boldsymbol{\nabla}^2 \Phi &= \frac{1}{R}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Phi(r) \\ &= \frac{32\pi^2 e}{3\,(2\pi\hbar)^3}\,(2me\Phi)^{3/2} \end{aligned} \tag{3.13}$$

solve numerically. boundary condition:

$$\phi(r) \to \frac{Ze}{r}, \quad \text{for } r \to 0 \tag{3.14a}$$

normalize

$$4\pi \int \mathrm{d}r\, \rho(r) r^2 = Z \tag{3.14b}$$

$\rightsquigarrow$ “radius” of atom (contains all but one electron)

$$\overline{R} \simeq \text{consanta} Z^{1/3} \tag{3.15}$$

3.3 The Hartree approximation

Assume

$$\psi(1 \dots N) = \varphi_1(1) \dots \varphi_N(N) \tag{3.16a}$$

as solution to

$$H\psi = E\psi \tag{3.16b}$$

with

$$H = \sum_i \left(\frac{p_i^2}{2m} - \frac{Ze^2}{r_i} \right) + \sum_{i>j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{3.16c}$$

let φ_i be distinct and orthogonal (partially taking into account Pauli principle) and normalized

$$\int \mathrm{d}^3 r_i \, |\varphi_i(r_i)|^2 = 1 \tag{3.17}$$

Want to find stationary state with respect to variation in φ_i taking into account normalization via Lagrange multipliers ε_i

$$\begin{aligned} \langle H \rangle = & \sum_i \int \mathrm{d}^3\mathbf{r} \left(\varphi_i^*(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 - \frac{Ze^2}{r} \right) \varphi_i(r) \right) \\ & + \sum_{i>j} \int \mathrm{d}^3\mathbf{r} \int \mathrm{d}^3\mathbf{r} \, \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \varphi_i(r) \varphi_j(r') \\ & + \sum_i \varepsilon_i \left(\int \mathrm{d}^3 r \, |\varphi_i(r)|^2 - 1 \right) \end{aligned} \tag{3.18}$$

take functional derivative $\frac{\delta}{\delta \varphi_i^*}$

$$\left(-\frac{\hbar}{2m} \nabla^2 - \frac{Ze^2}{r} \right) \varphi_i + V_i(r) \varphi_i(r) = \varepsilon_i \varphi_i(r) \tag{3.19a}$$

$$V_i(r) = \sum_{j \neq i} \int \mathrm{d}^3 r' \, \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \, |\varphi_j(\mathbf{r}')|^2 \tag{3.19b}$$

interaction of i-th electron with potential caused by all other ($j \neq i$) electrons ε_i: ionization energy of i-ith electron. "solve" numerically with iterative procedure. start with "guess" for $\varphi_i^{(0)}$. $\rightsquigarrow$ into Eq. 3.19b $\rightsquigarrow$ $V_i^{(0)}$ $\rightsquigarrow$ into Eq. 3.19a solve $\rightsquigarrow$ $\varphi_i^{(1)}$ $\rightsquigarrow$ etc.

physical interpretation of Lagrange multipliers $\varepsilon_i\ \varphi_i^* \cdot 3.19a$

$$\Rightarrow \int \mathrm{d}^3 r \left(\frac{-\hbar^2}{2m} \left|\nabla_i \varphi_i\right|^2 + \left(-\frac{Ze^2}{r_i} + V_i \right) \left|\varphi_i\right|^2 \right) = \varepsilon_i \tag{3.20a}$$

with ε_i the ionization energy of i-th electron, assuming others are not affected.

3.4 Hartree-Fock approximation

improved ansatz for

$$\psi\left(1, \ldots, N\right) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(1) & \cdots & \varphi_N(1) \\ \vdots & \ddots & \vdots \\ \varphi_1(N) & \cdots & \varphi_N(N) \end{vmatrix} \tag{3.21a}$$

fully comptible with Pauli $\rightsquigarrow$ as for Hartree, plug into H and minimize. Eq. 3.19a stayse the same. Eq. 3.19b

$$\begin{aligned} &\frac{1}{2} \sum_{j \neq i} \int \mathrm{d}^3 \mathbf{r}_i \int \mathrm{d}^3 \mathbf{r}_j \frac{e^2}{\left|\mathbf{r}_i - \mathbf{r}_j\right|} \\ &\quad \times \left(\varphi_i^*(r_i) \varphi_j^*(r_j) \varphi_i(r_i) \varphi_j(r_j) - \varphi_i^*(r_i) \varphi_j^*(r_j) \varphi_i(r_j) \varphi_j(r_i) \right) \end{aligned} \tag{3.22a}$$

with $\varphi_i^*(r_i)\varphi_j^*(r_j)\varphi_i(r_i)\varphi_j(r_j)$ the Hartree term and $\varphi_i^*(r_i)\varphi_j^*(r_j)\varphi_i(r_j)$ the exchange term.

To understand exchange term consider $N = 2$

$$\psi\left(1, 2\right) = \frac{1}{\sqrt{2!}} \left(\varphi_i(1) \varphi_2(2) - \varphi_1(2) \varphi_2(1) \right) \tag{3.23a}$$

"new" in H-F write down all terms for

$$\begin{aligned} \langle \psi | \frac{1}{\left|\mathbf{r}_1 - \mathbf{r}_2\right|} | \psi \rangle = \frac{1}{2} \int \mathrm{d}^3 \mathbf{r}_1 \int \mathrm{d}^3 \mathbf{r}_2 \, &(\varphi_1^*(r_1) \varphi_2^*(r_2) \varphi_1(r_1) \varphi_2(r_2) + \text{“}1 \leftrightarrow 2\text{”} \\ &- \varphi_1^*(r_1) \varphi_2^*(r_2) \varphi_1(r_2) \varphi_2(r_1) - \text{“}1 \leftrightarrow 2\text{”}) \end{aligned}$$

3.5 The periodic table and Hund's rules

Electron in atom feels effective potential V_{eff} (from nucleus and other electron) which is spherically symmetric.

$$\psi_i = R_{n\ell}(r) Y_\ell^m \left(\theta, \varphi\right) \chi_{m_s} \,, \tag{3.24a}$$

with χ_{m_s} the spin and $R_{n\ell}$ different from hydrogen

general rules

$$\begin{cases} n \text{ small} & \text{stronger binding} \\ \ell \text{ small} & \text{electron is closer to nucleus} \end{cases} \tag{3.25}$$

"compete sometimes". for each n :

$$\begin{array}{lllll} \ell & 0 & 1 & 2 & 3 \\ \text{name} & S & P & D & F \\ \deg 2\,(2\ell+1) & 2 & 4 & 6 & 10 \end{array} \tag{3.26a}$$

$$\begin{array}{lllcll} K\text{-shell} & n=1 & \ell=0 & 2 \text{ elements} & H, He & (1s) \\ L\text{-shell} & n=2 & \ell=0 & 2 & Li, Be & (2s) \\ & & \ell=1 & 6 & B-Ne & (2s) \\ M\text{-shell} & n=3 & \ell=0 & 2 & Na-Mg & (3s) \\ & & \ell=1 & 6 & Al-Ar & (3s) \\ & & \ell=2 & \dots & \dots & (3p) \\ N\text{-shell} & n=4 & \ell=0 & 2 & & (4s) \\ & n=3 & \ell=2 & 10 & Al-Ar & (3d) \\ & n=4 & \ell=1 & 6 & \dots & (4p) \end{array} \tag{3.26b}$$

configuration of electron $\rightarrow$ chemical properties of elements. What is the configuration (total spin, L, J) ofthe outer electron. $\rightarrow$ Hund's rules (empirical) [Notation ${}^{2s+1}L_J$]

Example 3.5.1: Carbon $(1s)^2\,(2s)^2\,(2p)^2$
for each of the 2 $2p$-electrons $2p$-electrons we can have $m_\ell = -1, 0, 1$, $m_s = -\frac{1}{2}, \frac{1}{2}$. $\rightarrow$ 6 possibilities
for both

$$\frac{6 \cdot 5}{2} = 15 \text{ possibilities} \tag{3.27}$$

$$L = \begin{array}{c} 0,2 \quad \text{symmetric} \\ 1 \ \text{anti-symmetric} \end{array} \tag{3.28a}$$

$$S = \begin{array}{c} 1 \quad \text{symmetric} \\ 0\text{anti-symmetric} \end{array} \tag{3.28b}$$

total wave function is antisymmetric

$$\begin{array}{ccccc} L & S & J & {}^{2s+1}L_J & \text{deg} \\ \hline 0 & 0 & 0 & {}^1S_0 & 1 \\ & & 0 & {}^3P_0 & 1 \\ 1 & 1 & 1 & {}^3P_1 & 3 \\ & & 2 & {}^3P_2 & 5 \\ 2 & 0 & 2 & {}^1D_2 & 5 \\ & & & & 15 \end{array} \tag{3.29}$$

Which one is ground state? $\rightarrow$ Hund's rules

(1) make spin maximal

$$\begin{aligned} &\rightarrow \text{spin part more symmetric} \\ &\rightarrow \text{orbital port more asymmetric} \\ &\rightarrow \text{electron further away from each other} \\ &\rightarrow \text{less repulsion} \end{aligned} \tag{3.30}$$

for C: $s = 1$

(2) make L maximal

$$\begin{aligned} &\rightarrow \text{electron average further away from each other} \\ &\rightarrow \text{less repulsion} \end{aligned} \tag{3.31}$$

no impaft for C

(3)

$$\Delta E_{\text{SO}} = \text{constant}\left(j\left(j+1\right) - \ell\left(\ell+1\right) - s\left(s+1\right)\right) \tag{3.32a}$$

$$\text{constant} \begin{cases} > 0 & \text{if subshell } \textit{no} \text{ more than half filled } J = |L - S| \\ < 0 & \text{if subshell more than half filled } J = |L + S| \end{cases} \tag{3.32b}$$

for C first case and

$$\begin{aligned} J &= |L - S| \\ &= 0 \end{aligned} \tag{3.33}$$

ground state ${}^3P_0$

Chapter 4

Approximation methods for time-dependent problems

We now want to know time evolution

$$|\psi(t)\rangle = U(t, t_0)\,|\psi(t_0)\rangle \tag{4.1}$$

We know:

$$i\hbar \frac{\partial}{\partial t}\,|\psi(t)\rangle = H(t)\,|\psi(t)\rangle \tag{4.2}$$

with $H(t)$ now time dependent $\to$ more complicated relation between H and U

4.1 Time-dependent perturbation theory

Let

$$H(t) = H_0 + \lambda V(t)\,, \tag{4.3a}$$

with H_0 time independent and that can be solved and $V(t)$ with t the "only" difference to chapter 1.

$$H_0 \left|\psi_n^{(0)}\right\rangle = E_n^{(0)} \left|\psi_n^{(0)}\right\rangle \tag{4.3b}$$

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\,|\psi(t)\rangle &= H(t)\,|\psi(t)\rangle \\ &= (H_0 + \lambda V(t))\,|\psi(t)\rangle \end{aligned} \tag{4.3c}$$

for any t:

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-\frac{i}{\hbar}E_n^{(0)}} \left|\psi_n^{(0)}\right\rangle \tag{4.3d}$$

$$\langle \psi(t) |\, \psi(t)\rangle = 1 \tag{4.3e}$$

$$\Rightarrow \sum_n |c_n|^2 = 1 \tag{4.3f}$$

we can also write

$$V(t)\left|\psi_n^{(0)}\right\rangle = \sum_m \left|\psi_m^{(0)}\right\rangle \left\langle\psi_m^{(0)}\right| V(t) \left|\psi_n^{(0)}\right\rangle \tag{4.3g}$$

with

$$\left\langle\psi_m^{(0)}\right| V(t) \left|\psi_n^{(0)}\right\rangle = V_{mn}(t) \tag{4.3h}$$

$\rightarrow$ into Schrödinger

$$\sum_n \left(i\hbar\dot{c}_n + E_n^{(0)} c_n\right)\left|\psi_n^{(0)}\right\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n^{(0)}t}\Bigg(E_n^{(0)}\left|\psi_n^{(0)}\right\rangle + \lambda\sum_m V_{mn}(t)\left|\psi_m^{(0)}\right\rangle\Bigg) \tag{4.3i}$$

swap labels m and n on rhs

$$\sum_n i\hbar\dot{c}_n e^{-\frac{i}{\hbar}E_n^{(0)}t}\left|\psi_n^{(0)}\right\rangle = \sum_{n,m}\lambda c_m e^{-\frac{i}{\hbar}E_m^{(0)}t} V_{nm}(t)\left|\psi_n^{(0)}\right\rangle \tag{4.3j}$$

$$\Rightarrow \dot{c_n} = (i\hbar)^{-1}\lambda\sum_m V_{mn} e^{\frac{i}{\hbar}\left(E_n^{(0)}-E_m^{(0)}\right)t} c_m \tag{4.3k}$$

with

$$\omega_{nm} = \frac{E_n^{(0)} - E_m^{(0)}}{\hbar} \tag{4.3l}$$

so

$$\dot{c_n} = (i\hbar)^{-1}\lambda\sum_m V_{nm} e^{i\omega_{nm}t} c_m\,. \tag{4.3m}$$

Now expand in λ ($\rightarrow$ perturbation theory)

$$c_n = c_n^{(0)} + \lambda c_n^{(1)} + \lambda^2 c_n^{(2)} + \dots \tag{4.3n}$$

$$\dot{c}_n^{(0)} = 0, \quad \mathcal{O}(\lambda^0) \tag{4.3o}$$

$$c_n^{(1)} = (i\hbar)^{-1}\sum_m V_{nm} e^{i\omega_{nm}t} c_m^{(0)} \tag{4.3p}$$

...

$$c_n^{(j)} = (i\hbar)^{-1}\sum_m V_{nm} e^{i\omega_{nm}t} c_m^{(j-1)} \tag{4.3q}$$

Let system be in state $\left|\psi_i^{(0)}\right\rangle$ at time to initial condition

$$c_m^{(0)} = \delta_{im} \tag{4.3r}$$
$$\dot{c}_f^{(1)} = (i\hbar)^{-1} V_{fi} e^{i\omega_{fi}t} \tag{4.3s}$$
$$c_f^{(1)}(t) = (i\hbar)^{-1} \int_{t_0}^{t} \mathrm{d}t' V_{fi}(t') e^{i\omega_{fi}t'} \tag{4.3t}$$

→ transition probability for the system to be found in state $\left|\psi_f^{(0)}\right\rangle$ at time t.

$$\begin{aligned} P_{i\,\to f} &= \left|c_f^{(1)}\right|^2 \\ &= \frac{1}{\hbar^2}\left|\int_{t_0}^{t} \mathrm{d}t'\; V_{fi} e^{i\omega_{fi}t'}\right|^2 + \mathcal{O}\left(\lambda^2\right) \end{aligned} \tag{4.3u}$$

approximation only valif if

$$\left|c_f\right|^2 \ll 1 \tag{4.3v}$$

Higher orders in λ will be covered section 4.4 and Exercise

4.2 Constant perturbation

Let

$$V(t) = \begin{cases} 0 & \text{for } t < t_0 (= 0) \\ V & \text{(constant) for } t > t_0 \end{cases} \tag{4.4a}$$

$$P_{i\,\to f} = \frac{1}{\hbar^2}\left|V_{fi}\right|^2 \left|\int_{t_0=0}^{t} \mathrm{d}t'\; e^{i\omega_{fi}t'}\right|, \tag{4.4b}$$

using

$$\begin{aligned} \int_{t_0\;=0}^{t} \mathrm{d}t'\; e^{i\omega_{fi}t'} &= \frac{2}{\omega^2}\left(1 - \cos\omega_{fi}t\right) \\ &= \frac{4}{\omega^2}\sin^2\left(\frac{\omega_{fi}t}{2}\right), \end{aligned} \tag{4.4c}$$

and

$$\begin{aligned} \delta_t(\alpha) &\equiv \frac{\sin^2\left(\alpha t\right)}{\pi\alpha^2 t} \\ &= \begin{cases} \frac{t}{\pi} & \alpha = 0 \\ < \frac{1}{\pi\alpha^2 t} & \alpha \neq = 0 \end{cases}, \end{aligned} \tag{4.4d}$$

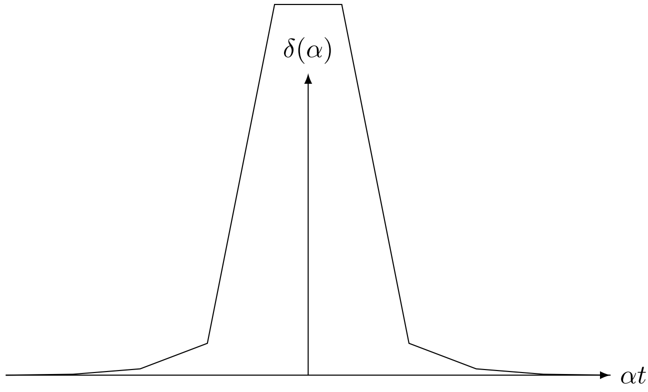

Figure 4.1:

which is plotted in Fig. 4.1

$$\lim_{t\to\infty} P_{i\to f} = \frac{\pi t}{\hbar^2} \left|V_{fi}\right|^2 \delta\left(\frac{E_f^{(0)} - E_j^{(0)}}{2\hbar}\right) \tag{4.4e}$$

$$P_{i\to f} = \frac{2\pi t}{\hbar} \left|V_{fi}\right|^2 \delta\left(E_f^{(0)} - E_i^{(0)}\right) \tag{4.4f}$$

transition rate= probability/time

$$\Gamma_{fi} = \frac{2\pi}{\hbar} \left|V_{fi}\right|^2 \delta\left(E_f - E_i\right) \tag{4.4g}$$

Consider transitions into continuous specturm $\rho(E)$

$$\int_{E_1}^{E_2} \mathrm{d}E\, \rho(E) = \text{number of states in energy range } E_1\text{-}E_2 \tag{4.5a}$$

$$\sum_f \Gamma_{fi} \to \int \mathrm{d}E\, \rho(E)\Gamma_{fi} = \frac{2\pi}{\hbar}\rho(E_f) \left|V_{fi}\right|^2 \tag{4.5b}$$

golden rule!

requires contiuum of states and applicabiliity of perturbation theory.

4.3 Periodic perturbations

Let

$$V(t) = \left(Ve^{-i\omega t} + V^\dagger e^{+i\omega t}\right), \quad \text{for } t > t_0 = 0 \tag{4.6}$$

The transition probability $P_{i\to f}$ is given by

$$\begin{aligned} P_{i\to f}(t) &= \frac{1}{\hbar}\left|\int_{t_0}^{t} \mathrm{d}t' \left(V_{fi}e^{i(\omega_{fi}-\omega)t'} + V^\dagger_{fi}e^{i(\omega_{fi}+\omega)t'}\right)\right|^2 \\ &= \frac{\pi t}{\hbar^2}\left(|V_{fi}|^2 \sin^2\left(\frac{t}{2}(\omega_{fi}-\omega)\right) + \left|V^\dagger_{fi}\right|^2 \frac{\sin^2\left(\frac{t}{2}(\omega_{fi}+\omega)\right)}{\pi t\left(\frac{\omega_{fi}+\omega}{2}\right)^2}\right. \\ &\qquad \left. + \Re\left(V_{fi}V^\dagger_{fi}\cdot\mathcal{F}(\omega_{fi},\omega)\right)\right) \end{aligned} \tag{4.7a}$$

with $\mathcal{F}(\omega_{fi},\omega)$ the interference pattern

the behaviour for large t, $t > \frac{2\pi}{\omega}$ (recall $\sin^2 \to \delta$-function), interference term vanishes, transition rate

$$\Gamma_{i\to f} = \frac{P_{i\to f}}{t}, \quad \text{for large } t \tag{4.8a}$$

$$\begin{aligned} \Gamma_{i\to f} &= \frac{2\pi}{\hbar}\left(|V_{fi}|^2\,\delta\left(\underbrace{E_f - E_i - \hbar\omega}_{E_f = E_i + \hbar\omega}\right)\right. \\ &\qquad \left. + \left|V^\infty_{fi}\right|^2\,\delta\left(\underbrace{E_f - E_i + \hbar\omega}_{E_f = E_i - \hbar\omega}\right)\right) \\ &= \text{absorption of } \hbar\omega + \text{emission of } \hbar\omega \end{aligned} \tag{4.8b}$$

$\to$ inteaction of matter with radiation

4.4 The Interaction picture

Consider again evolution operator

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle \tag{4.9}$$

i) $U(t, t_0) = \mathbf{1}$

ii) $U(t, t_1) U(t_1, t_0) = U(t, t_0)$

iii)

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle &= H(t) |\psi(t)\rangle \\
&= i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi(t_0)\rangle \\
&= H(t) U(t, t_0) |\psi(t_0)\rangle
\end{aligned}
\tag{4.10}
$$

U satisfies

$$
i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t) U(t, t_0) \tag{4.11a}
$$

Formial solution:

$$
U(t, t_0) = 1 + (i\hbar)^{-1} \int_{t_0}^{t} \mathrm{d}t' \, H(t') U(t', t_0) \tag{4.11b}
$$

"solve" by iteration

$$
\begin{aligned}
U(t, t_0) &= \sum_{n=0}^{\infty} U^{(n)}(t, t_0) \\
&= 1 + U^{(1)} + \dots
\end{aligned}
\tag{4.11c}
$$

$$
U^{(1)}(t, t_0) = (i\hbar)^{-1} \int_{t_0}^{t} \mathrm{d}t_1 \, H(t_1) \tag{4.11d}
$$

$$
\begin{aligned}
U^{(2)}(t, t_0) &= (i\hbar)^{-2} \int_{t_0}^{t} \mathrm{d}t_2 \, H(t_2) \int_{t_0}^{t} \mathrm{d}t_1 \, H(t_1) \\
&= \frac{(i\hbar)^{-2}}{2!} \int_{t_0}^{t} \mathrm{d}t_1 h \, \mathrm{d}t_2 \, T(H(t_1) H(t_2))
\end{aligned}
\tag{4.11e}
$$

(last step see exercise)

$$
\vdots = \vdots \tag{4.11f}
$$

$$
\begin{aligned}
U^{(n)}(t, t_0) &= (i\hbar)^{-n} \int_{t_0}^{t} \mathrm{d}t_n \, H(t_n) \int_{t_0}^{t_n} \mathrm{d}t_{n-1} \, H(t_{n-1}) \dots \int_{t_0}^{t_2} \mathrm{d}t_1 \, H(T_1) \\
&= \frac{1}{n!} (i\hbar)^{-n} \int_{t_0}^{t} \mathrm{d}t_n \int_{t_0}^{t} \mathrm{d}t_{n-1} \dots \int_{t_0}^{t} \mathrm{d}t_1 \, T(H(t_n) \dots H(t_1))
\end{aligned}
\tag{4.11g}
$$

with T the time ordering operator

$$T\left(H(t_1)\dots H\left(t_1\right)\right) = H\left(t_{\tau(1)}\dots H\left(t_{\tau(n)}\right)\right) \tag{4.11h}$$

if

$$\begin{aligned} t_{\tau(1)} &> t_{\tau(2)} \\ &> \dots \\ &> t_{\tau(n)} \end{aligned} \tag{4.11i}$$

full solution

$$U\left(t, t_0\right) = T\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,H(t')}\right] \tag{4.11j}$$

cannot be expanded in a useful way. *All terms are equally important.*

4.5 Dipole approximation and selection rules

Transitions are governed by $\alpha^* \langle\psi_0|\, j\left(\mathbf{k}\right)\cdot\boldsymbol{\epsilon}^*\left(\mathbf{k}\right)|\psi_n\rangle$

$$\begin{aligned} j\left(\mathbf{k}\right) &= \frac{1}{2m}\left(\mathbf{p}e^{-i\mathbf{k}\cdot\mathbf{r}}] + e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}\right) \\ &= \frac{\mathbf{p}}{m} \end{aligned} \tag{4.12a}$$

with Dipole approximation

$$e^{-i\mathbf{kr}} = 1 - i\mathbf{kr} + \dots \tag{4.12b}$$

$$k \sim \frac{1}{\lambda}, \quad \text{for visible light} \sim \left(10\times10^{-7}\,\mathrm{m}\right)^{-1} \tag{4.12c}$$

$$\begin{aligned} r &\sim \text{size of atom} \\ &\sim \text{Bohr radius} \\ &\sim 10\times10^{-10}\,\mathrm{m} \end{aligned} \tag{4.12d}$$

$$\begin{aligned} \mathbf{j}\cdot\mathbf{A} &\rightarrow \text{Dipole approx.} \\ :\mathbf{j} &= \frac{\mathbf{p}}{m} \end{aligned} \tag{4.12e}$$

(radiation filed $\sim$ constant within atom)

Aside: this is equivalent to a term

$$e\mathbf{r}\cdot\mathbf{E} = -\mathbf{d}\cdot\mathbf{E} \tag{4.12f}$$

with $\mathbf{d}$ dipole moment

$$\mathbf{d} \equiv -e\mathbf{r} \tag{4.12g}$$

(compare $\boldsymbol{\mu}\cdot\mathbf{B}$)

Proof:

$$\begin{aligned}[r_x, H_0] &= \left[r_x, \frac{\mathbf{p}^2}{2m}\right] \\ &= \frac{1}{2m}\left([r_x, \mathbf{p}]\,\mathbf{p} + \mathbf{p}\,[r_x, p]\right)\end{aligned} \tag{4.13a}$$

with

$$[r_x, \mathbf{p}] = \sum_y i\hbar\delta_{xy}p_y \tag{4.13b}$$

$$[r_x, H_0] = \frac{p_x}{m}i\hbar \tag{4.13c}$$

$$[r, H_0] = i\hbar\frac{\mathbf{p}}{m} \tag{4.13d}$$

emission

$$\begin{aligned}\langle\psi_0|\, e\mathbf{r}\cdot\mathbf{E}\,|\psi_n\rangle &= -\frac{e}{c}\langle\psi_0|\,\mathbf{r}\cdot\dot{\mathbf{A}}\,|\psi_n\rangle \\ &= -\frac{e}{c}i\omega\langle\psi_0|\,\mathbf{r}\cdot\mathbf{A}\,|\psi_n\rangle \\ &= -\frac{e}{c}\frac{i}{\hbar}\left(E_n - E_0\right)\langle\psi_0|\,\mathbf{r}\cdot\mathbf{A}\,|\psi_n\rangle \\ &= -\frac{e}{c}\frac{i}{\hbar}\langle\psi_0|\,[\mathbf{r}, H_0]\cdot\mathbf{A}\,|\psi_n\rangle\end{aligned} \tag{4.13e}$$

using Eq. 4.13d

$$\begin{aligned}\langle\psi_0|\, e\mathbf{r}\cdot\mathbf{E}\,|\psi_n\rangle &= -\frac{e}{c}\langle\psi_0|\,\frac{\mathbf{p}}{m}\cdot\mathbf{A}\,|\psi_n\rangle \\ &= \frac{e}{c}\langle\psi_0|\,\mathbf{j}\cdot\mathbf{A}\,|\psi_n\rangle\end{aligned} \tag{4.13f}$$

Proof (alternative): Make gauge trafo with

$$\chi(\mathbf{r}, t) = -\mathbf{A}(t)\cdot\mathbf{r} \tag{4.14a}$$

$$\mathbf{A} \to \mathbf{A} + \boldsymbol{\nabla}\xi = 0 \tag{4.14b}$$

$$0 = \Phi \to \Phi - \frac{1}{c}\dot{\chi} = -\frac{1}{c}\dot{\mathbf{A}}\cdot\mathbf{r} = -\mathbf{E}\cdot\mathbf{r} \tag{4.14c}$$

$$H - e\Phi = -e\mathbf{r}\mathbf{E} \tag{4.14d}$$

Atomic transitions are only possible if

$$\left\langle\psi_{n'\ell'm'_\ell}\middle|\,\mathbf{r}\,\middle|\psi_{n\ell m_\ell}\right\rangle \neq 0 \tag{4.15a}$$

Given ℓ, m_ℓ this imposes constraints on $\ell', m_{\ell'}$ $\rightarrow$ selection rules (in dipole approximation). Can be obtained by (solving at properties of spherical harmonics).

$$\int \mathrm{d}\Omega \, \left(Y_{\ell'}^{m_{\ell'}}(\theta,\phi)\right)^* \begin{pmatrix} x+iy \\ x-iy \\ z \end{pmatrix} \mathcal{Y}_\ell^{m_\ell}(\theta,\phi) \tag{4.16a}$$

this is most of the time 0 exept if

$$\left\langle \psi_{n'\ell'm'_\ell} \middle| z \middle| \psi_{n\ell m_\ell} \right\rangle \neq 0, \quad \ell' = \ell \pm 1, m'_\ell = m_\ell \tag{4.16b}$$

$$\left\langle \psi_{n'\ell'm'_\ell} \middle| x \pm iy \middle| \psi_{n\ell m_\ell} \right\rangle \neq 0, \quad \ell' = \ell \pm 1, m'_\ell = m_\ell \pm 1 \tag{4.16c}$$

(or use Wigner-Ekcart theorem, $\mathbf{r}$ is a vector operator)
$\Rightarrow$ selection rules for E_1 tronsitions (dipole approximation)

$$\Delta\ell = \pm 1 \tag{4.16d}$$

$$\Delta m = 0, \pm 1 \tag{4.16e}$$

These rules are violated by "beyound-dipole" transitions (e.g. E_2 quadrupole transitions).

Further selection rules: $\Delta S = 0$ (spin part of wavefunction not affected by $\mathbf{r} \cdot \mathbf{E}$) always true: *no* transitions between $j = 0 \rightarrow j = 0$ (total angular momentum conservation)

Chapter 5

Potential scattering

We consider

$$H = H_0 + V(r) \tag{5.1a}$$

with

$$\lim_{r \to \infty} rV(r) = 0, \quad \text{(i.e. } \textit{not} \text{ Coloumb)} \tag{5.1b}$$

V is restricted to "small" region.
Want to find stationary solutions

$$\psi(\mathbf{r}, t) = e^{-\frac{i}{\hbar}Et}\psi(\mathbf{r}), \quad \text{for } r \to \infty \tag{5.1c}$$

steady incoming beam scattered by potential (more general treatment in section 7)

5.1 Elastic scattering and cross sections

we are looking for solutions to

$$(H_0 + V)|\psi\rangle = E|\psi\rangle \tag{5.2a}$$

$$\begin{aligned} E_{\text{in}} &= E_{\text{out}} \\ &= \frac{p^2}{2m} \\ &= \frac{\hbar^2 k^2}{2m} \end{aligned} \tag{5.2b}$$

of the form

$$r \to \infty \tag{5.2c}$$

$$\begin{aligned} \psi_k(\mathbf{r}) &\to \psi_{\text{in}}(\mathbf{r}) + \psi_{\text{sc}}(\mathbf{r}) \\ &= e^{i\mathbf{kr}} + f(\theta, \phi)\frac{e^{ikr}}{r} \end{aligned} \tag{5.2d}$$

where we are not interested in $\psi(r)$ for small r (in range of V) and $f(\theta, \phi)$ is the scattering amplitude and $\frac{e^{ikr}}{r}$ is the outgoing spherical wave

Differential cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{N}{F} \tag{5.3}$$

N**:** #particles scattered into $\mathrm{d}\Omega$ per time in $N \, \mathrm{d}\Omega$

F**:** flux of incoming particles, number/time/unit area

Exercise: For $|\psi_{\text{in}}|^2 = 1$ (1 part/volume),

$$\begin{aligned} F &= V \\ &= \frac{p}{m} \\ &= \frac{\hbar k}{m} \end{aligned} \tag{5.4a}$$

outgoing:

$$\begin{aligned} \mathbf{j} &= \dots \\ &= \frac{\hbar k}{m} \left| f(\theta, \phi) \right|^2 \frac{\mathbf{e}_r}{r^2} \end{aligned} \tag{5.4b}$$

$$\Rightarrow \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left| f(\theta,' i) \right|^2 \tag{5.4c}$$

total cross section

$$\sigma = \int \mathrm{d}\Omega \, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \tag{5.4d}$$

5.2 Partial-wave analysis

For central potential $V(r)$. No ϕ dependence in ψ_k

$$\psi_k(r, \theta) = \sum_{\ell=0}^{\infty} R_\ell(kr) \, P_\ell(\cos\theta) \tag{5.5a}$$

$P_\ell(\cos\theta)$ being Legendre polynomials

$$f(\theta) = \sum_{\ell=0}^{\infty} P_\ell(k) \, P_\ell(\cos\theta) \tag{5.5b}$$

$\rightarrow$ equation for R_ℓ:

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\ell\,(\ell+1)}{r^2} + 2m\,(V(r)-E)\,R_\ell\,(kr) = 0 \tag{5.5c}$$

Aside: Assume V is constant ($\rho = kr$)

Solutions for $E > V$: Spherical Bessel function:

$$j_\ell\,(\rho) \equiv (-\rho)^\ell \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell \frac{\sin\rho}{\rho} \tag{5.6a}$$

Spherical Neumann function:

$$n_\ell\,(\rho) = -\,(-\rho)^\ell \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell \frac{\cos\rho}{\rho} \tag{5.6b}$$

$$j_\ell\,(\rho) \xrightarrow{\rho\,\to 0} \rho^\ell \xrightarrow{\rho\,\to\infty} \frac{1}{\rho}\sin\left(\rho - \frac{\pi\ell}{2}\right) \tag{5.7a}$$

$$n_\ell(\rho) \xrightarrow{\rho\,\to 0} \frac{1}{\rho^{\ell-1}} \xrightarrow{\rho\,\to\infty} -\frac{1}{\rho}\cos\left(\rho - \frac{\pi\ell}{2}\right) \tag{5.7b}$$

$$h_\ell = j_\ell \pm i n_\ell \tag{5.7c}$$

General solution for radial Schrödinger equation for $r \to 0$ $\frac{\ell(\ell+1)}{r^2}$ dominant for $V(r)$ less singular tan $\frac{1}{r^2}$

$$\begin{aligned} R_\ell(r) &\sim j_\ell(\rho) \\ &= j_\ell\,(kr) \end{aligned} \tag{5.8a}$$

for $r \to \infty$ $V(r) \to 0$ general solution

$$\begin{aligned} R_\ell(r) &= B_\ell(k) j_\ell(kr) + C_\ell n_\ell(kr) \xrightarrow{r\to\infty} B_\ell(k)\frac{1}{kr}\sin\left(kr - \frac{\pi\ell}{2}\right) \\ &\quad - C_\ell(k)\frac{1}{kr}\cos\left(kr - \frac{\pi\ell}{2}\right) \\ &= \frac{1}{kr}A_\ell(k)\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right), \\ &\quad A_\ell = \sqrt{B_\ell^2 + C_\ell^2},\ \text{phase shift } \tan\delta_\ell = -\tfrac{C_\ell(k)}{B_{\ell(k)}} \end{aligned} \tag{5.8b}$$

note: for $V = 0$:

$$R_\ell \sim j_\ell\,(kr) \tag{5.9a}$$

i.e. C_ℓ and $\delta_\ell = 0$

Solutions for $r \to \infty$ are characterized by phase shift δ_ℓ
Next: find relation between $\delta_\ell \leftrightarrow f(\theta)$

$$\psi_k \to e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)e^{ikr}\frac{1}{r} \tag{5.10}$$

central potential

$$\psi_k = \sum_{\ell=0}^{\infty} R_\ell\,(kr)\,P_\ell\,(\cos\theta) \tag{5.11a}$$

$$f_k = \sum_{\ell=0}^{\infty} f_\ell(k) P_\ell\,(\cos\theta) \tag{5.11b}$$

Schrödinger equation for R_ℓ, solution $\overset{r\to\infty}{\sim} j_\ell n_\ell$

$$\begin{aligned} R_\ell(kr) &\overset{r\to\infty}{\simeq} \frac{1}{kr}\left(B_\ell \sin\left(kr - \frac{\ell\pi}{2}\right) + C_\ell \cos\left(kr - \frac{\ell\pi}{2}\right)\right) \\ &= \frac{1}{kr} A_\ell \sin\left(kr - \frac{\ell\pi}{2} + \underbrace{\delta_\ell(k)}_{\text{phase shift}}\right) \end{aligned} \tag{5.11c}$$

for $V = 0$ we have $C_\ell = 0$, i.e. $\rho_\ell = 0$

next: find relation between phase shifts $\delta_\ell(k)$ and scattering amplitude $f(\theta)$ $\left(\to \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)$
Aside: ree particle eigenfunction in spherical coordinates

$$\psi_{j\ell m_\ell}\,(r,\phi,\theta) = C_{J\ell}(kr) Y_\ell^{m_\ell}\,(\theta,\phi)\,, \quad E = \tfrac{\hbar^2 k^2}{2m} \tag{5.12a}$$

Form a basis, expand

$$e^{i\mathbf{kr}} = e^{ikr\cos\theta} \tag{5.12b}$$

in this basis

$$e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty}\sum_{m_\ell}^{\ell} C_{\ell m_\ell} j_\ell\,(kr)\,Y_\ell^{m_\ell}\,(\theta,\phi) \tag{5.12c}$$

having no ϕ dependence

$$\rightsquigarrow e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty} a_\ell j_\ell(kr) P_\ell\,(\cos\theta) \tag{5.12d}$$

fix coefficient a_ℓ (use orthogonality)

$$e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell j_\ell(kr)\, P_\ell(\cos\theta) \tag{5.12e}$$

Put everything into (*) for $r \to \infty$

$$\frac{1}{kr} A_\ell \sin\left(kr - \frac{\pi\ell}{2} + \delta_\ell\right) = (2\ell+1)\, i^\ell \frac{1}{kr} \sin\left(kr - \frac{\pi\ell}{2}\right) + f_\ell \frac{e^{ikr}}{r} \tag{5.12f}$$

$$\begin{aligned} \frac{A_\ell}{2i} e^{ikr} e^{-\frac{i\pi\ell}{2}} e^{i\delta_\ell} - \frac{A_\ell}{2i} e^{-ikr} e^{\frac{i\pi\ell}{2}} e^{-i\delta_\ell} &= (2\ell+1)\, i^\ell \frac{1}{2i} e^{ikr} e^{-\frac{i\ell\pi}{2}} \\ &\quad - (2\ell+1)\, i^\ell \frac{1}{2i} e^{-ikr} e^{\frac{i\ell\pi}{2}} + k f_\ell e^{ikr} \end{aligned} \tag{5.12g}$$

$$A_\ell = (2\ell+1)\, i^\ell e^{i\delta_\ell} \tag{5.12h}$$

$$\begin{aligned} f_\ell &= \frac{2\ell+1}{2ik} \left(e^{2i\delta_\ell} - 1\right) \\ &= \frac{2\ell+1}{k} e^{i\delta_\ell} \sin(\delta_\ell) \end{aligned} \tag{5.12i}$$

having the full information of $f(\theta)$, thus $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$

$$\begin{aligned} f(\theta) &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} e^{i\delta_\ell} \sin(\delta_\ell)\, P_\ell(\cos\theta) \\ &= \sum_{\ell=0}^{\infty} f_\ell P_\ell(\cos\theta) \end{aligned} \tag{5.12j}$$

Total cross section

$$\begin{aligned} \sigma_{\text{tot}} &= \int \mathrm{d}\Omega\, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \\ &= \int \mathrm{d}\Omega\, |f(\theta)|^2 \\ &= 2\pi \int_{-1}^{1} \mathrm{d}\cos\theta \sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} f_\ell f_{\ell'}^* P_\ell(\cos\theta)\, P_\ell(\cos\theta) \end{aligned} \tag{5.13a}$$

use

$$\int \mathrm{d}\cos\theta\, P_\ell(\cos\theta)\, P_{\ell'}(\cos\theta) = \frac{2}{2\ell+1} \delta_{\ell\ell'} \tag{5.13b}$$

$$\begin{aligned}\Rightarrow \sigma_{\text{tot}} &= \sum_{\ell=0}^{\infty} 4\pi \frac{2\ell+1}{k^2} \sin^2\left(\delta_{/ell}\right) \\ &\equiv \sum_{\ell=0}^{\infty} \sigma_\ell\end{aligned} \tag{5.13c}$$

5.2.1 The optical theorem

$$\begin{aligned}\mathrm{im}\left(f\left(\theta=0\right)\right) &= \Im\left(\sum_{\ell=0}^{\infty} f_\ell\right) \\ &= \mathrm{im}\left(\sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} e^{i\delta_\ell} \sin\left(\delta_\ell\right)\right) \\ &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} \sin^2\left(\delta_\ell\right)\end{aligned} \tag{5.14a}$$

$$\begin{aligned}\Rightarrow \sigma_{\text{tot}} &= \frac{4\pi}{k} \mathrm{im}\left(f\left(\theta\right.\right. \\ &\left.\left.= 0\right)\right)\end{aligned} \tag{5.14b}$$

often an "easy" way to compute the total cross section by computing im of forward scattering amplitude.

Partial-wave useful if not too many σ_ℓ contribute.

semi-classical: potential of range A, $V(r) = 0$ for $r > 0$

classical: no scattering if $b > a$

$$\begin{aligned}L &\simeq \ell \cdot \hbar \\ &= b \cdot P \\ &= b \cdot \hbar \cdot k\end{aligned} \tag{5.15}$$

no scattering for

$$\begin{aligned}b &= \frac{\ell}{k} \\ &> a\end{aligned} \tag{5.16}$$

5.3 Coulomb scattering

So far we have assumed $\mathbf{r}V(\mathbf{r}) \to 0$, $|\mathbf{r}| \to \infty$, but this is not the case for Coulomb scattering.
However, exact solution is known (recall Hydrogen atom)

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \frac{Z_1 Z_2 e^2}{r}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{5.17}$$

- hydrogen $E < 0$ (bound states),

$$\lim_{r\to\infty} |\psi(\mathbf{r})|^2 = 0 \tag{5.18}$$

- scattering $E > 0$ with different

$$\nabla^2 = \frac{4}{\xi+\eta}\left(\partial_\xi \xi \partial_\xi + \partial_\eta \eta \partial_\eta\right) + \underbrace{\frac{1}{\xi\eta}\frac{\partial^2}{\partial\varphi^2}}_{\spadesuit} \tag{5.19}$$

$\spadesuit$: do not contribute → Confluent hypogeometric equation→
2 linearly independent solutions: find the linear combination which is regular at the origin. Result for $r \to \infty$

$$\gamma = \frac{m Z_1 Z_2 e^2}{\hbar^2 k} \tag{5.20a}$$

$$\begin{aligned}\psi_\ell(r) \xrightarrow[r\to\infty]{\mathbf{k}=k\mathbf{e}_z} &\underbrace{e^{i(kz+\gamma\log 2k(r-z))}}_{\text{distorted plane wave}} \\ &- \frac{\gamma}{2k\sin^2\frac{\vartheta}{2}}\frac{\Gamma(1+\gamma)}{\Gamma(1-i\gamma)}e^{-i\gamma\log\left(\sin\frac{2\vartheta}{2}\right)}\underbrace{\frac{e^{i(kr-\gamma\log 2kr)}}{2}}_{\text{distorted outgoing plane wave}}\end{aligned} \tag{5.20b}$$

This looks the same as

$$\psi(\mathbf{r}) = e^{i\mathbf{kr}} + f(\vartheta)\frac{e^{ikr}}{r} \tag{5.21}$$

but gets additional phases, because *not* $rV(r) \xrightarrow{r\to\infty}$ Cross-section

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= |f_c(\vartheta)| \\ &= \frac{\gamma}{4k^2 \sin^4 \frac{\vartheta}{2}} \\ &= \left(\frac{Z_1 Z_2 e^2}{4E}\right)^2 \frac{1}{\sin^4 \frac{\vartheta}{2}}\end{aligned} \tag{5.22}$$

$\to$ $\to$ Rutherford scattering formula (classical!)

$\to$ Phases drop out in this case

Additional phases can have an effect in scattering of 2 identical particles. Here $2 \to 2$, $\xrightarrow{A}\xleftarrow{B}$. Go to the center of mass frame (sec 2.1)

$$\left[-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{5.23}$$

- $$\begin{aligned}\mu &= \frac{m_1 m_2}{m_1 + m_2} \\ &= \frac{m}{2}, \quad \text{reduced mass}\end{aligned} \tag{5.24}$$

$$V \sim \text{interaction potential} \tag{5.25}$$

$$\begin{aligned}\mathbf{r} &= \mathbf{r}_A - \mathbf{r}_B \\ &\sim \text{relative coordinate}\end{aligned} \tag{5.26}$$

In QM the particles are undistinguishable when idential. Two pictures with a particle A and B going to each other.

Moreover: Total wave function (spin+space+...) must be either symmetric or antisymmetric under exchange $A \leftrightarrow B$, $\mathbf{r} \leftrightarrow -\mathbf{r}$. Spatial wave function

$$\psi_{\text{sym/antysym}} = \left(e^{i\mathbf{kr}} \pm e^{-i\mathbf{kr}}\right) + \left(f\left(\vartheta\right) \pm f\left(\pi - \vartheta\right)\right)\frac{e^{ikr}}{r} \tag{5.27}$$

Example: Coulomb scattering of two protons (spin $\frac{1}{2}$, fermions $\to$ t.w.f. antisymmetric). Let us look at unpolarized protons and assume that the potential does not depend on spin. Spin wave function:

prob $\frac{1}{4}$ singlet state (anti sym.)

prob. $\frac{3}{4}$ triplet states (sym.)

Spatial wave function

prob $\frac{1}{4}$ symm.

$$\to \sigma_{\text{sing}} = |f_\ell(\vartheta) + f_c(\pi - \vartheta)|^2 \tag{5.28}$$

prob $\frac{3}{4}$ antisym.

$$\to \sigma_{\text{trp}} = |f_c(\vartheta) - f_c(\pi - \vartheta)|^2 \tag{5.29}$$

Unpolarized cross-section:

$$\begin{aligned}\sigma &= \frac{1}{4}|f_c(\vartheta) + f(\pi-\vartheta)|^2 + \frac{3}{4}|f_c(\vartheta) - f_c(\pi-\vartheta)|^2 \\ &= |f_c(\vartheta)|^2 + |f_c(\pi-\vartheta)|^2 \\ &\quad -\frac{1}{2}\left(f_c(\vartheta)f_c^*(\pi-\vartheta) + f_c^*(\vartheta)f_c(\pi-\vartheta)\right) \overset{Z_1=Z_2=1}{=} \left(\frac{e}{4E}\right)^2 \left(\underbrace{\frac{1}{\sin\frac{4\theta}{2}} + \frac{1}{\cos^4\frac{\vartheta}{2}}}_{\text{classical}} \right. \\ &\qquad \left. - \frac{\cos\left(\gamma\log\left(\tan^2\frac{\vartheta}{2}\right)\right)}{\sin^2\frac{\vartheta}{2}\cos^2\frac{\vartheta}{2}}\right)\end{aligned} \tag{5.30}$$

Mott scattering formula

5.4 Lippman- Schwinger equation & Green's function

Again:

$$E_k = \frac{\hbar^2 k^2}{2m} \tag{5.31a}$$

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_k\right)\psi_k(\mathbf{r}) = V(\mathbf{r})\psi(\mathbf{r}) \tag{5.31b}$$

If we know the *Green's function* defined by

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_k\right) g_k(\mathbf{r}) = \delta(\mathbf{r}) \tag{5.32}$$

then we can write a formual solution for $\psi_k(\mathbf{r})$

$$\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} + \int \mathrm{d}^3\,\mathbf{r}' g_k(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{5.33}$$

with $e^{i\mathbf{kr}}$ solution to homogeneous equation ($V = 0$) Checik it at home.

Idea: As in section 4.4 we can turn this formal solution into a series for ψ_k (in powers of V)

First: Compute g_k: Go to Fourier space

$$g_k(\mathbf{r}) = \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} e^{-i\mathbf{qr}} \tilde{g}_k(\mathbf{q}) \tag{5.34}$$

We get

$$\begin{aligned}\left(\frac{\hbar^2}{2m}\nabla^2 + E_k\right) g_k(\mathbf{r}) &= \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3}\left(-\frac{\hbar^2}{2m}q^2 + \frac{\hbar^2}{2m}k^2\right) e^{-i\mathbf{qr}}\tilde{g}_k(\mathbf{q}) \\ &= \delta(\mathbf{r}) \\ &= \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} e^{-i\mathbf{qr}}\end{aligned} \tag{5.35a}$$

$$\begin{aligned}\Rightarrow \tilde{g}_k(\mathbf{q}) &= \frac{2m}{\hbar^2}\frac{1}{k^2-q^2} \\ &= \left(E_k - \frac{\hbar^2 q^2}{2m}\right)^{-1}\end{aligned} \tag{5.35b}$$

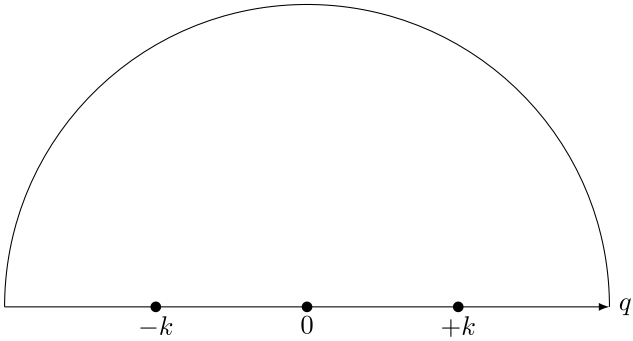

Figure 5.1:

$$
\begin{aligned}
g_k(r) &= \frac{1}{(2\pi)^3}\int_0^\infty \mathrm{d}q \int_0^{2\pi} |\mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}\cos\vartheta \\
&\qquad \cdot q^2 \frac{2m}{\hbar^2}\frac{1}{k^2-q^2} e^{-iqr\cos\vartheta} \\
&= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2} \\
&= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty \mathrm{d}q \frac{q^2}{iqr}\frac{1}{k^2-q^2}\left(e^{iqr} - \underbrace{e^{-iqr}}_{\spadesuit}\right) \\
&= \frac{m}{2\pi^2\hbar^2}\frac{1}{ir}\int_{-\infty}^{\infty}\mathrm{d}q \frac{q}{k^2-q^2} e^{iqr}
\end{aligned}
\tag{5.35c}
$$

$\spadesuit$:

$$
\int_0^\infty \mathrm{d}q \xrightarrow{q\ \rightarrow -1} -\int_0^{-\infty} = \int_{-\infty}^{0} \mathrm{d}q \tag{5.36}
$$

Integral is not well defined! $\rightarrow$ We need a prescription for the poles.
We use contour integral, close it in upper half plane

$$
\begin{aligned}
q &= q_{R\ell} + iq_{\ell m} \\
&\rightarrow e^{iqr} \\
&= e^{iq_{R\ell}r} e^{-q_{\ell m}r}
\end{aligned}
\tag{5.37}
$$

We deform the contour at $q = \pm k$ $\rightarrow$different options, giving *different asympt behaviours* for $g_k(\mathbf{r})$! For negative point outside and positive point inside curve:

$$g_k^+(r) = 2\pi i \frac{m}{2\pi^2\hbar^2}\frac{1}{ir} Res_{q=k}\frac{-q}{(q-k)(q+k)}e^{iqr} = -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r} \tag{5.38a}$$

For negative point inside and positive point outside curve:

$$g_k^-(r) = -\frac{m}{2\pi\hbar^2}\frac{e^{-ikr}}{r} \tag{5.38b}$$

for both points inside:

$$g_k^+(r) + g_k^-(r) \tag{5.38c}$$

Both points outside

$$0 \tag{5.38d}$$

$g_k^+ \sim$ outgoing spherical wave

$g_k^- \sim$ incoming spherical wave

What we need is g_k^+!

$$\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} - \int \mathrm{d}^3\mathbf{r}' \frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')\psi(\mathbf{r}') \tag{5.39}$$

Check asymptotic behaviour ($\mathbf{r}'V(\mathbf{r}') \to 0$)

$$\begin{aligned} |\mathbf{r}-\mathbf{r}'| &\xrightarrow{|\mathbf{r}|\to\infty} r\left(1 - \frac{r'}{r}\cos\vartheta + \mathcal{O}\left(\left(\frac{r'}{r}\right)\right)\right) \\ &= r - \frac{\mathbf{rr}'}{r'} \\ &= r - \hat{e}_r \cdot \mathbf{r}' \end{aligned} \tag{5.40a}$$

We get:

$$\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} - \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}' \frac{e^{ikre^{-ik\mathbf{e}_r\mathbf{r}'}}}{r} \times V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{5.40b}$$

...

5.5 The Born approximation

Formal solution

$$\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} + \int \mathrm{d}^3\mathbf{r}'\, g_k^+\left(\mathbf{r}-\mathbf{r}'\right) V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{5.41a}$$

$$g_k^+\left(\mathbf{r}-\mathbf{r}'\right) = -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \tag{5.41b}$$

$$f = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}' e^{-ik\mathbf{e}_r\cdot\mathbf{r}'} V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{5.41c}$$

Solve this “pertubatively” by iteration.

$$\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{n=1}^{\infty}\int \mathrm{d}^3\mathbf{r}'\, K_(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'} \tag{5.42a}$$

$$K_1\left(\mathbf{r},\mathbf{r}'\right) = g_k^+\left(\mathbf{r}-\mathbf{r}'\right) V(\mathbf{r}'), \quad \sim V^1 \tag{5.42b}$$

$$\begin{aligned} K_n\left(\mathbf{r},\mathbf{r}'\right) &= \int \mathrm{d}^3\mathbf{r}''\, K_1\left(\mathbf{r},\mathbf{r}''\right) K_{n-1}\left(\mathbf{r}'',\mathbf{r}'\right), \quad \sim V^n \\ &= \int\left(\prod_{i=1}^{n}\mathrm{d}^3\mathbf{r}_i\right) g_k^+\left(\mathbf{r}-\mathbf{r}\right) V(\mathbf{r}_n) g^+\left(\mathbf{r}_n-\mathbf{r}_{n-1}\right)\dots g_k^+\left(\mathbf{r}_2\right. \\ &\qquad \left. -\,\mathbf{r}_1\right) V(\mathbf{r}_1) \end{aligned} \tag{5.42c}$$

Retaining only the 1st term we have (1st) Born approx.

$$\psi_k^{(1)}(\mathbf{r}) = e^{ikz}\underbrace{-\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}' V(\mathbf{r}')e^{ik(\mathbf{e}_z-\mathbf{e}_r)\cdot\mathbf{r}'}}_{f^{(1)}(\theta,\phi)}\frac{e^{ikr}}{r} \tag{5.43}$$

assuming k is along the z-axis. $f^{(1)}$ is the Fourier transform of potential w.r.t. $\mathbf{q}$

$$\begin{aligned} \mathbf{q} &\equiv k\left(\mathbf{e}_z-\mathbf{e}_r\right) \\ &= \mathbf{k}-\mathbf{k}', \quad \text{momentum transfer} \end{aligned} \tag{5.44a}$$

for central potential $V(r')$ (not $V(\mathbf{r}')$).

$$
\begin{aligned}
f^{(1)}(\theta,\phi) &= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}\phi \int_{-1}^{1} \mathrm{d}\cos\vartheta \int \mathrm{d}r'\, V(r') e^{iqr'\cos\vartheta} \\
&= -\frac{m}{\hbar^2}\int r'^2\,\mathrm{d}r'\,\frac{2\sin(qr')}{qr'}V(r')
\end{aligned}
\tag{5.45a}
$$

$$
f^{(1)}(\theta) = -\frac{2m}{\hbar^2 q}\int \mathrm{d}r'\, r' V(r')\sin\left(qr'\right), \quad q = 2k\sin\tfrac{\theta}{2}
\tag{5.45b}
$$

Note $f^{(1)}$ is real! Cp optical theorem!?

Example: Yukawa potential:

$$
V(r) = V_0\frac{e^{-\mu r}}{r}, \quad \mu \sim \text{range of interaction}
\tag{5.46a}
$$

$$
\begin{aligned}
f^{(1)} &= -\frac{2m}{\hbar^2 q}V_0 \underbrace{\int_0^\infty \mathrm{d}r' e^{-\mu r'}\sin(qr')}_{q/(\mu^2+q^2)} \\
&= -\frac{2m}{\hbar^2}\frac{V_0}{\mu^2+q^2}
\end{aligned}
\tag{5.46b}
$$

$$
\begin{aligned}
\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(1)} &= \left|f^{(1)}(\theta)\right|^2 \\
&= \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{\left(\mu^2+2k^2\left(1-\cos\theta\right)\right)^2}
\end{aligned}
\tag{5.46c}
$$

total cross section

$$
\begin{aligned}
\sigma^{(1)}_{\text{tot}} &= 2\pi\int_{-1}^{1}\mathrm{d}\!\cos\theta\left(\frac{2mV_0}{\hbar^2}\right)^2\frac{1}{\left(\mu^2+2k^2\left(1-\cos\theta\right)\right)^2} \\
&= 2\pi\left(\frac{2mV_0}{\hbar^2}\right)\frac{2}{\mu^4+4k^2\mu^2}
\end{aligned}
\tag{5.46d}
$$

Take limit $\mu \to 0$: "infinite" range of interaction

$$
V(\mathbf{r}) = \frac{V_0}{r}, \quad \text{(Coulomb)}
\tag{5.47a}
$$

$$
\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(1)}_{\text{Coulomb}} = \left(\frac{2mV_0}{\hbar^2}\right)^2\frac{1}{\left(2k^2\left(1-\cos\theta\right)\right)}
\tag{5.47b}
$$

but total cross section diverges!
Note $\lim_{r\to\infty} rV(r) \neq 0$ for Coulomb!

Chapter 6

General scattering theory

General scattering more complicated than in section 6 e.g. production of new particles. Want to use general representation, so $|\psi\rangle$ is a general state in Hilbert space (not nec. wave function)

6.1 Dynamics of scattering

Start from time dependent Schrödinger

$$i\hbar\partial_t |\psi, t\rangle = H |\psi, t\rangle \tag{6.1a}$$

$$H = H_0 + V \tag{6.1b}$$

$$\ldots = \ldots \tag{6.1c}$$

$$\begin{aligned}(i\hbar\partial_t - H_0) |\psi, t\rangle &= V |\psi, t\rangle \\ &= |\chi, t\rangle\end{aligned} \tag{6.1d}$$

Definition 6.1.1: Green operation $G_0(t, t')$ through

$$(i\hbar\partial_t - H_0) G_0(t, t') = \delta(t - t') \cdot \mathbf{1}, \quad (\leftarrow \text{operators}) \tag{6.2}$$

inhomogeneous differential equation in t

$$G_0^+(t, t') = -\frac{i}{\hbar}\theta(t - t') e^{-\frac{i}{\hbar}H_0(t-t')} \tag{6.3a}$$

$$G_0^-(t, t') = +\frac{i}{\hbar} \tag{6.3b}$$

Proof:

$$
\begin{aligned}
i\hbar\partial_t G_0^+\left(t-t'\right) &= i\hbar\left(-\frac{i}{\hbar}\right)\partial_t\theta\left(t-t'\right)e^{-\frac{i}{\hbar}H_0\left(t-t'\right)} \\
&= \delta\left(t-t'\right)e^{-\frac{i}{\hbar}H_0\left(t-t'\right)} \\
&\quad + \theta\left(t-t'\right)\left(-\frac{i}{\hbar}H_0\right)e^{-\frac{i}{\hbar}H_0\left(t-t'\right)} \\
&= \delta\left(t-t'\right) + H_0 G_0^+\left(t-t'\right)
\end{aligned} \tag{6.4a}
$$

Note: The superscripts $\pm$ are related to those in section 6

$$
G_0^{\pm}\left(t,t'\right) = G_0^{pm}\left(t-t'\right) \tag{6.5a}
$$

Write solution to Schrödinger

$$
\left|\psi^{\pm},t\right\rangle = \left|\psi^0,t\right\rangle + \int \mathrm{d}t' G_0^{\pm}\left(t-t'\right)V\left|\psi^{\pm},t'\right\rangle \tag{6.5b}
$$

with $\left|\psi^0,t\right\rangle$ solution to homogeneous problem

$$
\left(i\hbar\partial_t - H_0\right)\left|\psi_0,t\right\rangle = 0 \tag{6.5c}
$$

The "physical" solution is given by $\left|\psi^+,t\right\rangle$, since $G^+\left(t-t'\right)$ moves "forward" in time. (retardation)
To make connection with section 6: $t \to E$

$$
\begin{aligned}
G_0^+\left(E\right) &= \int_{-\infty}^{\infty}\mathrm{d}t\, e^{\frac{i}{\hbar}Et}G_0^+(t) \\
&= -\frac{i}{\hbar}\int_0^{\infty}\mathrm{d}t\, e^{\frac{i}{\hbar}Et}e^{-\frac{i}{\hbar}H_0 t}
\end{aligned} \tag{6.6a}
$$

with

$$
G_0^+(t) = G_0^+\left(t,t'=0\right) \tag{6.6b}
$$

for $t \to \infty$ need $E \to E + i0^+, 0^+ > 0$

$$
\begin{aligned}
G_0^{\pm} &= \frac{1}{E - H_0 \pm i0^+} \\
&\equiv \left(E - H_0 \pm i0^+\right)^{-1}
\end{aligned} \tag{6.6c}
$$

$|\psi^{\pm}, t\rangle$ evolves with H, but was equal to free state $\left|\psi^{0}, t\right\rangle$ @ $t \to -\infty$
Let α be a complete set of quantum number of H_0 (including E_α)

$$\to \left|\psi_\alpha^0, t\right\rangle \leftrightarrow \left|\psi_\alpha^{\pm}, t\right\rangle \tag{6.7a}$$

make Fourier $t \to E$ of Eq. $\pm$

$$\begin{aligned}\underbrace{\int \mathrm{d}t\, e^{\frac{i}{\hbar}Et}\left|\psi_\alpha^{\pm}, t\right\rangle}_{\left|\psi_\alpha^{\pm}(E)\right\rangle \to \left|\psi_\alpha^{\pm}\right\rangle} &= \underbrace{\int \mathrm{d}t\, e^{\frac{i}{\hbar}Et}\left|\psi_\alpha^{0}, t\right\rangle}_{\left|\psi_\alpha^{0}(E)\right\rangle \sim \left|\psi_\alpha^{0}\right\rangle} \\ &\quad + \int \mathrm{d}t\, e^{\frac{i}{\hbar}Et} \underbrace{\int \mathrm{d}t'\, G_0^{\pm}\left(t-t'\right)}_{t \to t+t'} V\left|\psi_\alpha^{\pm}, t\right\rangle\end{aligned} \tag{6.7b}$$

$$\int \mathrm{d}t\, e^{\frac{i}{\hbar}Et} G_0^{+}(t) = G_0^{+}(E) \tag{6.7c}$$

$$V\left|\psi_\alpha^{\pm}(E)\right\rangle = \int \mathrm{d}t'\, e^{\frac{i}{\hbar}Et'} V\left(\psi_\alpha^{\pm}(E)\right) \tag{6.7d}$$

$$\left|{}^{\pm}_{\alpha}\right\rangle = \left|\psi_\alpha^0\right\rangle + G_0^{\pm} V\left|\psi_\alpha^{\pm}\right\rangle, \quad \text{(Lippmann-Schwinger)} \tag{6.8a}$$

Solution:

$$\begin{aligned}\left|\psi_\alpha^{\pm}\right\rangle &= \left(1 - G_0^{\pm}V\right)^{-1}\left|\psi_\alpha^0\right\rangle \\ &= \frac{1}{\left(G_0^{\pm}\right)^{-1} - V}\left(G_0^{pm}\right)^{-1}\left|\psi_\alpha^0\right\rangle \\ &= \frac{1}{E_\alpha - H_0 \pm i0^{+} - V}\left(E_{?a} - H_0 \pm i0^{+} - V + V\right)\left|\psi_\alpha^0\right\rangle \\ &= \underbrace{\frac{1}{E_\alpha - H \pm i0^{+}}}_{G^{\pm}E_\alpha}\left(E_\alpha - H + V \pm i0^{+}\right)\left|\psi_\alpha^0\right\rangle \\ &= \left(1 + G^{\pm}V\right)\left|\psi_\alpha^0\right\rangle \\ \psi_\alpha^{\pm} &= \left(1 + G^{\pm}V\right)\left|\psi_\alpha^0\right\rangle\end{aligned} \tag{6.9a, 6.9b}$$

can also be obtained from (exercise 2)

$$\left|\psi^{\pm}, t\right\rangle = \lim_{t' \to \mp\infty} i\hbar G^{+}\left(t-t'\right)\left|\psi_0, t'\right\rangle \tag{6.9c}$$

6.2 Møller operators & scattering operator

α: Complete set of quantum numbers

$$H_0 \left|\psi_\alpha^0\right\rangle = E_\alpha \left|\psi_\alpha^0\right\rangle \tag{6.10a}$$

$$H \left|\psi_\alpha^\pm\right\rangle = E_\alpha \left|\psi_\alpha^\pm\right\rangle \tag{6.10b}$$

Consider again

$$\begin{aligned}\left|\psi_\alpha^\pm\right\rangle &= \left|\psi_\alpha^0\right\rangle + \left(E_\alpha - H_0 + \pm O^+\right)^{-1} V \left|\psi_\alpha^\pm\right\rangle \\ &= \left|\psi_\alpha^0\right\rangle + \int \mathrm{d}\beta \, \frac{T_{\beta\alpha}\left|\psi_\beta^0\right\rangle}{E_\alpha - E_\beta \pm i0^+}\end{aligned} \tag{6.10c}$$

$$1 = \int \mathrm{d}\beta \left|\psi_\beta^0\right\rangle\!\left\langle\psi_\beta^0\right| \tag{6.10d}$$

$$T_{\beta\alpha} \equiv \left\langle\psi_\beta^0\right| V \left|\psi_\alpha^\pm\right\rangle \tag{6.10e}$$

Transfer matrix

This state satisfies:

$$\int \mathrm{d}\alpha \, e^{-\frac{i}{\hbar}E_\alpha\tau} f(\alpha) \left|\psi_\alpha^\pm\right\rangle \xrightarrow{\tau \to \mp\infty} \int \mathrm{d}\alpha \, e^{-\frac{i}{\hbar}E_\alpha\tau} f(\alpha) \left|\psi_\alpha^0\right\rangle \tag{6.11a}$$

or

$$e^{-\frac{i}{\hbar}H\tau} \int \mathrm{d}\alpha \, f(\alpha) \left|\psi_\alpha^\pm\right\rangle \xrightarrow{e^{-\frac{i}{\hbar}H_0\tau}} \int \mathrm{d}\alpha \, f(\alpha) \left|\psi_\alpha^0\right\rangle \tag{6.11b}$$

$$\begin{aligned}\Rightarrow \left|\psi_\alpha^\pm\right\rangle &= \lim_{\tau\mp\infty} e^{+\frac{i}{\hbar}H\tau} e^{-\frac{i}{\hbar}H_0\tau} \left|\psi_\alpha^0\right\rangle \\ &= \Omega^\pm \left|\psi_\alpha^0\right\rangle\end{aligned} \tag{6.11c}$$

with $\Omega^\pm$ Møller operators

Typical scattering experiment:

At $t \to -\infty$ prepare state with quantum number α of H_0

Q: What is amplitude for this state to end up in (another) eigenstate of H_0 with quantum number β.

A:

$$\left\langle \psi_\beta^- \middle| \psi_\alpha^+ \right\rangle = \left\langle \psi_\beta^0 \right| \left(\Omega^-\right)^\dagger \Omega^+ \left| \psi_\alpha^0 \right\rangle \\ \equiv \left\langle \psi_\beta^0 \right| S \left| \psi_\alpha^0 \right\rangle \tag{6.12}$$

$$\begin{aligned} S &= \lim_{\substack{\tau\to\infty \\ \tau\to-\infty}} e^{\frac{i}{\hbar}H_0\tau} e^{\frac{i}{\hbar}H(\tau_0-\tau)} e^{-\frac{i}{\hbar}H_0\tau_0} \\ &= \lim_{\substack{\tau\to\infty \\ \tau_0\to-\infty}} U(\tau,\tau_0) \\ &= U(\infty,-\infty) \end{aligned} \tag{6.13}$$

ex 1: sheet 6:

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}\tau}U(\tau,\tau_0) &= e^{\frac{i}{\hbar}H_0\tau}\left(H-H_0\right)e^{\frac{i}{\hbar}H(\tau_0-\tau)}e^{-\frac{i}{\hbar}H_0\tau_0} \\ &= \underbrace{e^{\frac{i}{\hbar}H_0\tau} V e^{-\frac{i}{\hbar}H_0\tau}}_{V(\tau)} U(\tau,\tau_0) \\ &= V(\tau)U(\tau,\tau_0) \end{aligned} \tag{6.14a}$$

$V(\tau)$ evolution operator in IA picture section 4.4. Solution

$$U(\tau,\tau_0) = T\left(e^{-\frac{i}{\hbar}\int_{\tau_0}^{\tau} V(\tau)\,\mathrm{d}\tau}\right) \tag{6.15a}$$

and

$$\begin{aligned} S &= U(\infty,-\infty) \\ &= \mathbf{1} - \frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t_1 V(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_{-\infty}^{\infty}\mathrm{d}t_1 \int_{-\infty}^{t_1}\mathrm{d}t_2 V(t_1)V(t_2) + \dots \end{aligned} \tag{6.15b}$$

Note:

$$SS^\dagger = \mathbf{1}, \quad S \text{ operator is unitary} \tag{6.16}$$

S-matrix

$$\begin{aligned} S_{\beta\alpha} &\equiv \left\langle \psi_\beta^0 \right| S \left| \psi_\alpha^0 \right\rangle \\ &= \left\langle \psi_\beta^- \middle| \psi_\alpha^\dagger \right\rangle \end{aligned} \tag{6.17}$$

option 1 insert S operator

1st term:

$$\left\langle\psi_\beta^0\right| \mathbf{1} \left|\psi_\alpha^0\right\rangle = \delta\left(\beta-\alpha\right) \tag{6.18}$$

2nd term

$$\begin{aligned}
&-\frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t_1 \left\langle\psi_\beta^0\right| e^{\frac{i}{\hbar}H_0 t} V e^{-\frac{i}{\hbar}H_0 t}\left|\psi_\alpha^0\right\rangle \\
&= -\frac{i}{\hbar}\int \mathrm{d}t e^{-\frac{i}{\hbar}(E_\alpha-E_\beta)t}\left\langle\psi_\beta^0\right| V \left|\psi_\alpha^0\right\rangle \\
&= -2i\pi\delta\left(E_\alpha-E_\beta\right)V_{\beta\alpha}
\end{aligned} \tag{6.19}$$

3rd and 4th $\rightarrow$ exercise sheet 8

$$\begin{aligned}
\left|\psi_\alpha^\pm\right\rangle &= \left|\psi_\alpha^0\right\rangle + G_0^\pm(E)V\left|\psi_\alpha^\pm\right\rangle \\
&= \left|\psi_\alpha^0\right\rangle + G^\pm(E)V\left|\psi_\alpha^0\right\rangle
\end{aligned} \tag{6.20a}$$

$$\begin{aligned}
S_{\beta\alpha} &= \left\langle\psi_\beta^- \middle| \psi_\alpha^+\right\rangle \\
&= \left\langle\psi_\beta^0\right| S \left|\psi_\alpha^0\right\rangle
\end{aligned} \tag{6.20b}$$

6.3 structure of S-matrix

$\rightarrow$ exercise 3 sheet 8

$$\begin{aligned}
\left|\psi_\alpha^-\right\rangle - \left|\psi_\alpha^+\right\rangle &= G^- \\
&= \left(G^-(E_\alpha)-G^+(E_\alpha)\right)V\left|\psi_0^\alpha\right\rangle
\end{aligned} \tag{6.21a}$$

$$\left\langle\psi_\alpha^-\right| - \left\langle\psi_\alpha^+\right| = \left\langle\psi_\alpha^0\right| V\left(G^+(E_\alpha)-G^-\left(E_\alpha\right)\right) \tag{6.21b}$$

$$\begin{aligned}
S_{\beta\alpha} &= \left\langle\psi_\alpha^+\middle|\psi_\alpha^+\right\rangle \\
&= \left(\left\langle\psi_\beta^+\right| + \left\langle\psi_\beta^0\right| V\left(\frac{1}{E_\beta-H+i0^+}-\frac{1}{E_\beta-H-i0^+}\right)\right)\left|\psi_\alpha^+\right\rangle \\
&= \delta\left(\beta-\alpha\right) + \underbrace{\left(\frac{1}{E_\beta-E_\alpha+i0^+}-\frac{1}{E_\beta-E_\alpha-i0^+}\right)}_{\spadesuit}
\end{aligned} \tag{6.21c}$$

$$\spadesuit : \lim_{0+\searrow 0} \frac{-2i0^+}{\left(E_\beta - E_\alpha\right)^2 + \left(0^+\right)^2} \tag{6.21d}$$
$$= -2i\pi\delta\left(E_\beta - E_\alpha\right)$$

$$\delta(x) = \lim_{\varepsilon\searrow} \frac{1}{\pi} \frac{\varepsilon}{x^2 + \varepsilon^2} \tag{6.21e}$$

Remark 6.3.1:

$$\begin{aligned}\sqrt{H}\left|\phi\right\rangle &= \sum \sqrt{E} c_\alpha \left|\psi_\alpha\right\rangle \\ &= \sum c_\alpha \sqrt{E_\alpha} \left|\psi_\alpha\right\rangle\end{aligned} \tag{6.22a}$$

with

$$\left|\phi\right\rangle = \sum c_\alpha \left|\psi_\alpha\right\rangle, \tag{6.22b}$$

$$H\left|\psi_\alpha\right\rangle = E_\alpha \left|\psi_\alpha\right\rangle, \tag{6.22c}$$

$$\Rightarrow \sqrt{H}\left|\psi_\alpha\right\rangle = \sqrt{E_\alpha}\left|\psi_\alpha\right\rangle. \tag{6.22d}$$

$$S_{\beta\alpha} = \delta\left(\beta - \alpha\right) - 2i\pi\delta\left(E_\alpha - E_\beta\right) \underbrace{\left\langle\psi_\beta^0\right| V \left|\psi_\alpha^+\right\rangle}_{T_{\beta\alpha}\ \text{transition matrix}} \tag{6.23a}$$

Chapter 7

Quantization of radiation field

7.1 Quantization of free radiation field

from section 5.1

$$\mathbf{A}(\mathbf{r},t) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{\lambda} \left(\alpha(k\lambda)\, \boldsymbol{\epsilon}(k\lambda)\, e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} \right. \tag{7.1a}$$
$$\left. + \alpha^*(k,\lambda)\, \boldsymbol{\epsilon}^*(k,\lambda)\, e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega_k t} \right), \quad \omega = c\,|\mathbf{k}|$$

with $\lambda \to 2$ polarizations, $\boldsymbol{\epsilon}$ polarization vectors with

$$\mathbf{k}\cdot\boldsymbol{\epsilon}(k,\lambda) = 0 \tag{7.1b}$$

consider time dependence of single mode $(\mathbf{k},\lambda)$:

$$q_{k\lambda} = \alpha(k,\lambda)\, e^{-i\omega_k t} \tag{7.2a}$$
$$\ddot{q}_{k\lambda} = \omega_k^2 q_{k\lambda} \tag{7.2b}$$

$\rightarrow$ harmonics oscillator

Recall QMI: harmonic oscillator

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right) \tag{7.3a}$$

states

$$\hat{a}\,|0\rangle = 0 \tag{7.3b}$$
$$|n\rangle \equiv \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}\,|0\rangle \tag{7.3c}$$

The Hilbert space

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1}\, |n+1\rangle \dots \tag{7.3d}$$

$$\hat{N} = \hat{a}^\dagger \hat{a} \tag{7.3e}$$

with

$$\hat{N} |n\rangle = n\, |n\rangle\,, \quad \text{etc.} \tag{7.3f}$$

outlook $\mathbf{A} \to \hat{\mathbf{A}}$ (2nd quantization)

To motivate the interpretation of $\mathbf{A}$ as collection of independent harmonic oscillator compute

$$H = \frac{1}{8\pi} \int \mathrm{d}^3\mathbf{r}\, \left(\mathbf{E}^2 + \mathbf{B}^2\right) \tag{7.4a}$$

$$\begin{aligned} \mathbf{E} &= -\frac{1}{c}\dot{\mathbf{A}} \\ &= \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \sum_\lambda \left(\alpha \boldsymbol{\epsilon} \frac{i\omega}{c} e^{-i\omega t + i\mathbf{k}\cdot\mathbf{r}} - \alpha^* \boldsymbol{\epsilon} \frac{i\omega}{c} e^{i\omega t - i\mathbf{k}\mathbf{r}} \right) \end{aligned} \tag{7.4b}$$

$$\begin{aligned} \int \mathrm{d}^3\mathbf{r}\mathbf{E}^2 = &\int \mathrm{d}^3\mathbf{r} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{\lambda\lambda'} \left(\alpha\boldsymbol{\epsilon} e^{-i\omega t + i\mathbf{k}\mathbf{r}} - \alpha^* \boldsymbol{\epsilon}^* e^{i\omega t - i\mathbf{k}\mathbf{r}}\right) \left(\frac{i\omega}{c}\right) \\ &\cdot \left(\alpha' \boldsymbol{\epsilon}' e^{i\omega' t + i\mathbf{k}'\cdot\mathbf{r}} - \alpha^{*\prime} \boldsymbol{\epsilon}^{*\prime} e^{i\omega' t - i\mathbf{k}'\cdot\mathbf{r}}\right) \left(\frac{i\omega'}{c}\right) \\ = &\int \mathrm{d}^3\mathbf{r} \iint \sum_{\lambda\lambda'} \left(\alpha\alpha' \boldsymbol{\epsilon} \times \boldsymbol{\epsilon}'^* \frac{-\omega\omega'}{c^2} e^{-it\left(\omega-\omega'\right)} e^{r\mathbf{r}\left(\mathbf{k}-\mathbf{k}'\right)} \right) \end{aligned} \tag{7.4c}$$

use

$$\int \mathrm{d}^3\mathbf{r}\; e^{i\mathbf{r}\left(\mathbf{k}-\mathbf{k}'\right)} = (2\pi)^3\, \delta\left(\mathbf{k}-\mathbf{k}'\right) \tag{7.4d}$$

$$\int \frac{\mathrm{d}^3 k}{(2\pi)^3} \sum_{\lambda\lambda'} \left(\alpha\alpha' \boldsymbol{\epsilon} \times \boldsymbol{\epsilon}^{*\prime} \left(\frac{-\omega^2}{c^2}\right) + \dots \right) \tag{7.4e}$$

$$P = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \sum_\lambda \hbar \mathbf{k} a^*_{k\lambda} a_{k,\lambda} \tag{7.5a}$$

2nd quantiziation: so far $\mathbf{A}$ classical field, $a^* = f^{\text{cts}}$

$$A.H, P \to \hat{A}, \hat{H}, \hat{P} \tag{7.6a}$$

commutation relations

$$\begin{aligned}\left[\hat{a}_{k\lambda}, \hat{a}_{k'\lambda'}\right] &= \left[\hat{a}^{!}_{k\lambda}, \hat{a}^{\dagger}_{k'\lambda'}\right] \\ &= 0\end{aligned} \tag{7.6b}$$

$$\left[\hat{a}_{k\lambda}, \hat{a}^{\dagger}_{k'\lambda'}\right] = (2\pi)^3 \, \delta\left(k - k'\right) \delta_{\lambda\lambda'} \tag{7.6c}$$

k **continuous** $\to$ world in a box $\to$ k discrete; box $\to \infty$, $k \to$ const

λ**:** discrete

another way to quanise field $\mathbf{A}$:

$$\begin{aligned}\mathcal{L} &= \frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu} \\ &= \frac{1}{8\pi}\left(E^2 - B^2\right)\end{aligned} \tag{7.7a}$$

define conjugate momentum field.

$$\begin{aligned}\pi &= \frac{\partial f}{\partial \mathbf{A}} \\ &= \dots \\ &= -\frac{1}{4\pi c}\mathbf{E}^2\end{aligned} \tag{7.7b}$$

$A, \pi \to \hat{A}, \hat{\pi}$

$$\begin{aligned}\left[A_i\left(x,t\right), A_j\left(y,t\right)\right] &= \left[\pi_i\left(x,t\right), \pi_j\left(y,t\right)\right] \\ &= 0\end{aligned} \tag{7.8a}$$

$$\left[A_i, \pi_j\right] \approx i\hbar\delta\left(x - y\right)\delta_{ij} \tag{7.8b}$$

$$\begin{aligned}\mathbf{A}\left(\mathbf{r}, t\right) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \sum_{\lambda} \Big(&\alpha\left(k,\lambda\right) \boldsymbol{\epsilon}\left(k,\lambda\right) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} \\ &+ \alpha^*\left(\mathbf{k},\lambda\right) \boldsymbol{\epsilon}^*\left(\mathbf{k},\lambda\right) e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega t}\Big)\end{aligned} \tag{7.9a}$$

$$H = \frac{1}{8\pi}\int \mathrm{d}^3\mathbf{r}\,\left(\mathbf{E}^2 + \mathbf{B}^2\right) \tag{7.9b}$$

$$\int d^3\mathbf{r}\,\mathbf{E}^2 = \int d^3\mathbf{r} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \int \frac{d^3\mathbf{k}‘}{(2\pi)^3} \sum_{\lambda\lambda'} \Big(\alpha\alpha' \boldsymbol{\epsilon}$$
$$\cdot\, \boldsymbol{\epsilon} \left(-\frac{\omega\omega'}{c^2}\right) e^{-i(\omega+\omega')t} e^{+i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}}$$
$$+\, \alpha^*\alpha'^* \boldsymbol{\epsilon}^* \boldsymbol{\epsilon}'^* \left(-\frac{\omega\omega'}{c^2} e^{+i(\omega+\omega')t} e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}}\right)$$
$$-\, \alpha\alpha'^* \boldsymbol{\epsilon}^* \boldsymbol{\epsilon}'^* \left(-\frac{\omega\omega'}{c^2} e^{-i(\omega+\omega')t} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\right)$$
$$-\, \alpha^*\alpha' \boldsymbol{\epsilon}^* \boldsymbol{\epsilon}'^* \left(-\frac{\omega\omega'}{c^2} e^{+i(\omega+\omega')t} e^{+i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}}\right)\Big)$$
$$= \int \frac{d^3k}{(2\pi)^3} \sum_{\lambda\lambda'} \left(-\frac{\omega^2}{c^2}\right) \Big(\alpha_k\alpha_{-k} \boldsymbol{\epsilon}_k \cdot \boldsymbol{\epsilon}_{-k} e^{-2i\omega t} + \alpha_k^*\alpha_{-k}^* \boldsymbol{\epsilon}_k^*$$
$$\cdot\, \boldsymbol{\epsilon}_{-k}^* e^{2i\omega t} - \alpha_k\alpha_{+k}^* \boldsymbol{\epsilon}_k \cdot \boldsymbol{\epsilon}_k^* - \alpha_k^*\alpha_k \boldsymbol{\epsilon}_k^* \cdot \boldsymbol{\epsilon}_k$$
$$= \int \frac{d^3k}{(2\pi)^3} \sum_{\lambda} \left(\frac{\omega^2}{c^2}\right) \Big(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k$$
$$+ \left\{\alpha_k\alpha_{-k}, \alpha_k^*\alpha_{-k}^* \text{ terms}\right\}\Big)\Big)$$

use

$$\int d^3r\, e^{i(k\pm k')r} = (2\pi)^3 \delta(k \pm k') \tag{7.9c}$$

λ, k' integration and $\omega_{-k} = \omega_k = \omega$

$$\rightsquigarrow \int d^3v\,\mathbf{E}^2 = \frac{1}{(2\pi)^3} \int d^3k \left(-\frac{\omega^2}{c^2}\right) \big(\alpha_k\alpha_{-k} \boldsymbol{\epsilon}_k \boldsymbol{\epsilon}_{-k} e^{-2i\omega t} \tag{7.9d}$$
$$+ \alpha_k^*\alpha_{-k}^* \boldsymbol{\epsilon}_k^* \boldsymbol{\epsilon}_k^* e^{2i\omega t} - \alpha_k\alpha_k^* \boldsymbol{\epsilon}_k \boldsymbol{\epsilon}_k^* - \alpha_k^*\alpha_{+k} \boldsymbol{\epsilon}_k^* \boldsymbol{\epsilon}_k \big)$$

$$\begin{aligned} \int d^3\mathbf{r}\,\mathbf{B}^2 &= \dots \\ &= \int \frac{d^3k}{(2\pi)^3} \sum_{\lambda} \left(\frac{\omega^2}{c^2}\right) \left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k - \{\cdots\}\right) \end{aligned} \tag{7.9e}$$

$$H = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{\lambda} \frac{\omega^2}{4\pi c^2} \left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right) \tag{7.9f}$$

define:

$$\alpha^*(k,\lambda) = \sqrt{\frac{\omega}{2\pi c^2 \hbar}}\alpha^*(k,\lambda) \tag{7.10a}$$

$$\mathbf{A}(\mathbf{r},t) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\sqrt{\frac{2\pi c^2\hbar}{\omega}}\sum_\lambda \left(q_{k\lambda}\boldsymbol{\epsilon}_{k\lambda}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + q^*_{k\lambda}\boldsymbol{\epsilon}^*_{k\lambda}e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\right) \tag{7.10b}$$

$$H = \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\sum_\lambda \frac{\hbar\omega}{2}\left(a^*_{k\lambda}a_{k\lambda} + a_{k\lambda\lambda}a^*_{k\lambda}\right) \tag{7.10c}$$

$$\mathbf{P} = \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\sum_\lambda \hbar\mathbf{k}a^*_{k\lambda}a_{k\lambda} \tag{7.10d}$$

7.1.1 2nd quantization

So far $\mathbf{A}$ classical field, $a^{(*)}$ functions

$$a(k,\lambda) \to \hat{a}(k,\lambda), \quad \text{operator} \tag{7.11a}$$

$$a^*(k,\lambda) \to \hat{a}^\dagger(k,\lambda), \quad \text{operator} \tag{7.11b}$$

as for harmonic oscillator

$$\mathbf{A}, H, \mathbf{P} \to \hat{\mathbf{A}}, \hat{H}, \hat{P} \tag{7.11c}$$

commutation relations:

$$\left[\hat{a}_{k\lambda}, \hat{a}_{k',\lambda'}\right] = \left[\hat{a}^{k\lambda}_\dagger, \hat{a}^\dagger_{k',\lambda'}\right] \tag{7.12a}$$
$$= 0$$

$$\left[\hat{a}_{k\lambda}, \hat{a}^\dagger_{k'\lambda'}\right] = (2\pi)^3\,\delta\left(\mathbf{k}, -\mathbf{k}'\right)\delta_{\lambda\lambda'} \tag{7.12b}$$

k: continuous label → ften system in a box, k becomes discrete

λ: discrete, l.z

another way to quantize field $\mathbf{A}$

$$\mathcal{L} = \frac{1}{16\pi}F_{\mu\nu}F^{\mu\nu}$$
$$= \frac{1}{8\pi}\left(\mathbf{E}^2 - \mathbf{B}^2\right) \tag{7.13a}$$

define conjugate momentum field

$$\begin{aligned}\pi &= \frac{\partial f}{\partial \mathbf{A}} \\ &= \dots \\ &= -\frac{1}{4\pi c}\mathbf{E}^2\end{aligned} \tag{7.13b}$$

$A, \pi \to \hat{A}, \hat{\pi}$

$$[A_i(x,t), A_j(y,t)] = [\pi_i(x,t), \pi_j(y,t)] \tag{7.13c}$$
$$= 0$$
$$[A_i, \pi_j] \approx i\hbar\delta(x-y)\delta_{ij} \tag{7.13d}$$

7.2 Fock space

Built up as for single harmonic oscillator with "ladder" operators

$$\hat{a}^\dagger(k,\lambda) = \hat{a}^\dagger_{k\lambda}, \quad \text{creation operator} \tag{7.14a}$$

$$\hat{a}(k,\lambda) = \hat{a}_{k\lambda}, \quad \text{annihilation operator} \tag{7.14b}$$

start with vacuum $|0\rangle$ definition

$$\hat{a}_{k\lambda}|0\rangle = 0 \tag{7.14c}$$

$$|1(k,\lambda)\rangle = \hat{a}^\dagger|0\rangle \tag{7.14d}$$

state with 1 photon momentum, $\mathbf{k}$, polarization λ

General state Note:

$$\begin{aligned}&\hat{a}^\dagger_{k_j\lambda_j}|n_1(k_1,\lambda_1)\dots n_j(k_j,\lambda_j)\dots n_m(k_m,\lambda_m)\rangle \\ &\quad = \sqrt{n_j+1}\,|n_1\dots n_{j+1}\dots n_m\rangle\end{aligned} \tag{7.15a}$$

$$\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\sum_\lambda \hat{a}_{k\lambda}|n_1(k_1,\lambda_1)\rangle = \frac{1}{\sqrt{n_1!}}\int \frac{\mathrm{d}^3 k}{(2\pi)^3}\sum_\lambda \hat{a}_{k\lambda}\left(\hat{a}^\dagger_{k_1\lambda_1}\right)^{n_1}|0\rangle \tag{7.15b}$$

with

$$\hat{a}_{k\lambda}\left(\hat{a}^\dagger_{k_1\lambda_1}\right)^{n_1}|0\rangle = \left(\hat{a}^\dagger_{k_1\lambda_1}\right)^{n_1-1} n_1\left[\hat{a}_{k\lambda}, \hat{a}^\dagger_{k_1\lambda_1}\right] + \left(\hat{a}^\dagger_{k_1\lambda_1}\right)\hat{a}_{k\lambda} \tag{7.15c}$$

with

$$\left[\hat{a}_{k\lambda}, \hat{a}^{\dagger}_{k_1\lambda_1}\right] = n_1 \left(2\pi\right)^3 \delta\left(\mathbf{k} - \mathbf{k}_1\right) \delta_{\lambda\lambda_1} \tag{7.15d}$$

$$\begin{aligned}
\rightsquigarrow \int \frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3} \sum_{\lambda} \hat{a}_{k\lambda} \left|n_1\left(k_1, \lambda_1\right)\right\rangle &= \frac{n_1}{\sqrt{n_1!}} \left({}^{\dagger}_{k_1\lambda_1}\right)^{n_1-1} \left|0\right\rangle \\
&= \frac{n_1\sqrt{\left(n_1-1\right)!}}{\sqrt{n_1!}} \frac{\left(\hat{a}^{\dagger}_{k_1\lambda_1}\right)^{n_1-1}}{\sqrt{\left(n_1-1\right)!}} \left|0\right\rangle \\
&= \sqrt{n_1} \left|\left(n_1-1\right)\left(k_1\lambda_1\right)\right\rangle
\end{aligned} \tag{7.15e}$$

General:

$$\int \frac{\mathrm{d}^3 k}{\left(2\pi\right)^3} \sum_{\lambda} a_{k\lambda} \left|n_1 \dots n_m\right\rangle = \sum_{i=1}^{m} \sqrt{n_i} \left|n_1 \dots n_{i-1}, \dots n_m\right\rangle \tag{7.16a}$$

Compute expectation value of $\hat{H}$ in state $\left|n_1\left(k_1\lambda_1\right)\right\rangle$

$$\left\langle n_1\right| \hat{H} \left|n_1\right\rangle = \int \frac{\mathrm{d}^3 k}{\left(2\pi\right)^3} \sum_{\lambda} \frac{\hbar\omega}{2} \left\langle n_1\right| \hat{a}^{\dagger}_{k\lambda}\hat{a}_{k\lambda} + \underbrace{\hat{a}_{k\lambda}\hat{a}^{\dagger}_{k\lambda}}_{\hat{a}^{\dagger}_{k\lambda}\hat{a}_{k\lambda}} + \delta(0) \left|n_1\right\rangle \tag{7.16b}$$

$$\begin{aligned}
\left\langle n_1\right| \hat{H} \left|n_1\right\rangle &= \int \frac{\mathrm{d}^3 k}{\left(2\pi\right)^3} \sum_{\lambda} \hbar\omega \left\langle n_1\right| \hat{a}^{\dagger}_{k\lambda}\hat{a}_{k\lambda} \left|n_1\right\rangle \\
&= \hbar\omega \left\langle n_1\right| \hat{a}^{\dagger}_{k_1\lambda_1} \left|n_1 - 1\right\rangle \sqrt{n_1} \\
&= \hbar\omega n_1 \left\langle n_1 \middle| n_1\right\rangle \\
&= n_1 \hbar\omega
\end{aligned} \tag{7.16c}$$

$$\to \left\langle n_1 \dots n_m\right| \hat{H} \left|n_1 \dots n_m\right\rangle = \sum_{i=1}^{m} \hbar\omega_i n_i \tag{7.16d}$$

introduce interactions with matter (compare Section 5)

$$V = -\frac{q}{2mc}\left(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}\right) + \frac{q^2}{2mc^2}\hat{\mathbf{A}}^2 \tag{7.17a}$$

in Coulomb gauge

$$\boldsymbol{\nabla}\cdot\mathbf{A} = 0 \tag{7.18a}$$

$$\Rightarrow \mathbf{p}\cdot\mathbf{A} = \mathbf{A}\cdot\mathbf{p} \tag{7.18b}$$

$$\hat{V} = -\frac{q_-}{mc} p\cdot\hat{A} + \frac{q^2}{2mc^2}\hat{A}^2 \tag{7.18c}$$

is operator in Fock space and will be used to compute transition matrix elements

$$V_{\beta\alpha} = \left\langle \psi^0_\beta \right| V \left| \psi^0_\alpha \right\rangle \tag{7.18d}$$

7.3 Photon emission and absorption

We have considered these processes before in section 5.2

$$\begin{aligned} H &= H_0 + H_{\text{em}} + \hat{V} \\ &= \sum_i \frac{p_i^2}{2m} + \frac{1}{8\pi} \int \mathrm{d}^3 r \left(\hat{\mathbf{E}}^2 + \hat{\mathbf{B}}^2 \right) \\ &\quad + \text{interaction matter} \leftrightarrow \text{photons} \end{aligned} \tag{7.19a}$$

$$\begin{aligned} \text{eigenstates } \left| \psi^0_\alpha \right\rangle &= \left| \text{matter} \right\rangle \otimes \left| \text{photons} \right\rangle \\ &= \text{wave function} \otimes \text{new, Fockspace} \\ &= \left| A; n_1 \left(k, \lambda_1 \right) \dots n_m \left(k_m, \lambda_m \right) \right\rangle \end{aligned} \tag{7.19b}$$

7.3.1 Absorption of photon

$$V_{\beta\alpha} = \left\langle B; (n-1)\,(k,\lambda) \right| \hat{V} \left| A; n\,(k,\lambda) \right\rangle \tag{7.20a}$$

with

B**:** final state of atom

$(n-1)$**:** one photon “lost”

A**:** initial state of atom

$n\,(k,\lambda)$**:** n photons, k, λ

$$\begin{aligned} \rightsquigarrow V_{\beta\alpha} &= \frac{e}{mc} \int \frac{\mathrm{d}^3 \mathbf{k}}{(2\pi)^3} \sum_{\lambda'} \sqrt{\frac{2\pi\hbar c^2}{\omega'}} \\ &\quad \cdot \left\langle B; (n-1)\,(k,\lambda) \right| \hat{a}\,(k',\lambda')\, \mathbf{p} \cdot \boldsymbol{\epsilon}\,(k',\lambda')\, e^{i\mathbf{k}'\cdot\mathbf{r}} \left| A, n\,(k,\lambda) \right\rangle \end{aligned} \tag{7.20b}$$

$\hat{a}^\dagger$ term gives no contribution

$$\begin{aligned} \rightsquigarrow V_{\beta\alpha} &= \frac{e}{m} \sqrt{\frac{2\pi\hbar}{\omega}} \sqrt{n} \left\langle B; \right| \mathbf{p} \cdot \boldsymbol{\epsilon}(k,\lambda) e^{i\mathbf{k}\cdot\mathbf{r}} \left| A \right\rangle \\ &\sim \sqrt{n} \end{aligned} \tag{7.20c}$$

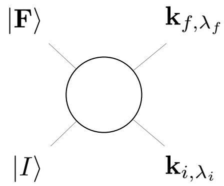

Figure 7.1:

7.3.2 Emission of photons

$$V_{\beta\alpha} = \langle B; (n+1)\,(k,\lambda)|\,\hat{V}\,|A; n\,(k,\lambda)\rangle\,, \tag{7.21a}$$

with $\hat{V}$ now anly $\hat{a}^\dagger$ part contribution.

$$\begin{aligned}\rightsquigarrow V_{\beta\alpha} &= \frac{e}{m}\sqrt{\frac{2\pi\hbar}{\omega}}\sqrt{n+1}\,\langle B|\,\mathbf{p}\cdot\boldsymbol{\epsilon}^*\,(k,\lambda)\,e^{-i\mathbf{k}\cdot\mathbf{r}}\,|A\rangle \\ &\sim \sqrt{n+1}\end{aligned} \tag{7.21b}$$

Note: This is non-zero even for $n = 0 \rightarrow$ spontaneous emission!
recall classical:

$$\Gamma_{n0} = \Gamma_{0n} \tag{7.22a}$$

$$\text{absorption} = \text{emission} \tag{7.22b}$$

now

$$\frac{\Gamma_{n0}}{\Gamma_{0n}} = \frac{n_{k\lambda}}{n_{k\lambda}+1} \tag{7.22c}$$

7.4 Scattering of photons by atoms

involves creation and annihilation of photon need $\hat{a}^\dagger\,(k_f,\lambda_f)\,\hat{a}\,(k_i,\lambda_i)$ recall

$$\hat{V} = \frac{e}{mc}\mathbf{p}\cdot\hat{\mathbf{A}} + \frac{e^2}{2mc^2}\hat{\mathbf{A}}^2 \tag{7.23}$$

where $\hat{\mathbf{A}}$ contains either $\hat{a}^\dagger$ or $\hat{a}$ and cotributes only at 2nd order, $\hat{\mathbf{A}}^2$ contains $\hat{a}^\dagger\hat{a} \rightarrow$ contributes at first order. Both $\hat{\mathbf{A}}$ and $\hat{\mathbf{A}}^2$ are $\sim \frac{e^2}{c^2}$

first-order contribution

$$
\begin{aligned}
V^{(1)}_{\beta\alpha} &= \langle F, 1\left(k_f, \lambda_f\right)| \frac{e^2}{2mc^2} \hat{\mathbf{A}}^2 \left|I, 1\left(k_i, f_i\right)\right\rangle \\
&= \frac{e^2}{2mc^2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{\left(2\pi\right)^3} \sum_{\lambda\lambda'} \frac{2\pi\hbar c^2}{\sqrt{\omega\omega'}} \\
&\quad \cdot \langle F, 1\left(k_f, \lambda_f\right)| \left(\hat{a}\boldsymbol{\epsilon} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + \hat{a}^\dagger\left(k,\lambda\right) e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\right) \\
&\quad \cdot \left(\hat{a}'\left(k',\lambda'\right) e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + \hat{a}^{\dagger\prime}\boldsymbol{\epsilon}'^{*} e^{-i\mathbf{k}\cdot\mathbf{r}+i'wt}\right) \left|I, 1\left(k_i, \lambda_i\right)\right\rangle \\
&= \frac{e^2}{2mc^2} \frac{2\pi\hbar c^2}{\sqrt{\omega_i\omega_f}} 2 \cdot \langle F| \boldsymbol{\epsilon}\left(k_i, \lambda_i \cdot \boldsymbol{\epsilon}\left(k_f, \lambda_f\right) e^{it(\omega_i-\omega_f)}\right) e^{i\mathbf{r}\cdot(\mathbf{k}_i-\mathbf{k}_f)} \left|I\right\rangle
\end{aligned}
\tag{7.24}
$$

Recall from section 7.2

$$
H = H_0 + V \tag{7.25a}
$$

$$
\begin{aligned}
S_{\beta\alpha} &= \delta\left(\beta-\alpha\right) - \frac{i}{\hbar} \int_{\mathbb{R}} \mathrm{d}t_1\, e^{-\frac{i}{\hbar}t_1(E_\alpha-E_\beta)} \left\langle \psi^0_\beta \right| V \left|\psi^0_\alpha\right\rangle \\
&\qquad - \frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t_1\, e^{-\frac{i}{\hbar}t_1(E_I+\hbar\omega_i-E_F-\hbar\omega_f)} \left(\frac{2e^2\hbar\pi}{m\sqrt{\omega_i\omega_f}} \boldsymbol{\epsilon} \right. \\
&\qquad\qquad \left. \cdot\, \boldsymbol{\epsilon}^* \left\langle F\right| \ldots \left|F\right\rangle \right)
\end{aligned}
\tag{7.25b}
$$

golden rule (sec 4.2/4.3) Transition rate $\frac{2\pi}{\hbar}\left|T\right|^2\rho$ cross section $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ (final photon energy $\hbar\omega_f + a\left(\hbar\omega_f\right)$)

- divide by flux $v = c$ (section 6.1)
- nr. states

$$
\begin{aligned}
\frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3} &= \frac{k^2\,\mathrm{d}k\,\mathrm{d}\Omega}{\left(2\pi\right)^3} \\
&= \frac{\omega_f^2\,\mathrm{d}\Omega}{\left(2\pi\right)^3 c^3\hbar} \mathrm{d}(\hbar\omega_f)
\end{aligned}
\tag{7.26a}
$$

$$
\rho\left(\omega_f\right) = \frac{\omega_f^2\,\mathrm{d}\Omega}{\left(2\pi\right)^3 c^3\hbar} \tag{7.26b}
$$

Feynman diagrams

Figure 7.2:

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{1}{c}\frac{2\pi}{\hbar}\underbrace{\frac{\omega_f^2}{(2\pi)^3 c^3\hbar}}_{\rho(\omega_f)}|T|^2 \\ &= \frac{e^4}{m^2c^4}\frac{\omega_f}{\omega_i}\left|\boldsymbol{\epsilon}_i\cdot\boldsymbol{\epsilon}_f^*\left\langle F\right| e^{i\mathbf{r}\cdot(\mathbf{k}_i-\mathbf{k}_f)}\left|I\right\rangle\right|^2\end{aligned} \tag{7.27a}$$

$$\left(\frac{\alpha\hbar}{mc}\right)^2 = r_0^2 \tag{7.27b}$$

(classical electron radius)

However, there are further contributions of order $\alpha^2 \sim e^4$ golden rule (sec 4.2/4.3) Transition rate $\frac{2\pi}{\hbar}|T|^2\rho$
cross section $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ (final photon)...

7.4.1 2nd order contribution

for $T_{\beta\alpha}$

$$S_{\beta\alpha} = \ldots\left(-\frac{i}{\hbar}\right)^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\sum_\gamma e^{-\frac{i}{\hbar}t_1(E_\gamma-E_\beta)}e^{-\frac{i}{\hbar}t_2(E_\alpha-E_\gamma)}V_{\beta\gamma}V_{\gamma\alpha} \tag{7.28a}$$

In our case

$$\begin{aligned}&\left(-\frac{i}{\hbar}\right)^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\sum\!\!\!\!\!\!\int \mathrm{d}N\, e^{-\frac{i}{\hbar}(E_N-E_F)t_i}e^{-\frac{i}{\hbar}(E_I-E_N)t_2}\left(\frac{e}{mc}\right)^2 \\ &\cdot\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\sum_{\lambda\lambda'}\left\langle F, P(\omega_f,\lambda_f)\right|\hat{a}_k\mathbf{p}\cdot\boldsymbol{\epsilon}_k e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t_1+\hat{a}_k^\dagger\mathbf{p}\cdot\boldsymbol{\epsilon}_k^* e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t_1}}\left|N\right\rangle \\ &\cdot\left\langle N\right|\hat{a}_{k'}\mathbf{p}\cdot\boldsymbol{\epsilon}_{k'}e^{i\mathbf{k}'\cdot\mathbf{r}-i\omega' t_2}+\hat{a}_{k'}^\dagger\mathbf{p}\cdot\boldsymbol{\epsilon}_{k'}^* e^{-i\mathbf{k}' j\mathbf{r}+i\omega' t_2}\left|I,1(k_i,\lambda_i)\right\rangle\end{aligned} \tag{7.29a}$$

need 1 $\hat{a}(k_i, \lambda_i)$ and one $\hat{a}^\dagger(k_f, \lambda_f)$

$$
\begin{aligned}
&= \dots \\
&= \langle F| \hat{a}^\dagger_{k_f} \dots |N\rangle \langle N| \dots \hat{a}_{k_i} |I\rangle + \langle F| \hat{a}_{k_i} \dots |N\rangle \langle N| \dots \hat{a}^{k_f}_{\dagger} |I\rangle
\end{aligned} \tag{7.29b}
$$

Kramers Heisenberg formula

$$
\begin{aligned}
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{\alpha\hbar}{mc}\right)^2 \frac{\omega_f}{\omega_i} \Bigg| &\boldsymbol{\epsilon}_i \boldsymbol{\epsilon}^*_f \delta_{FI} + \sum_N \langle F| \mathbf{p}\cdot\epsilon^*_f |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}_i |I\rangle \\
&+ \frac{\langle F| \mathbf{p}\cdot\boldsymbol{\epsilon}_i |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}^*_f |I\rangle}{m\left(E_I - \hbar\omega_f - E_N\right)} \Bigg|
\end{aligned} \tag{7.30}
$$

$\rightarrow$ limiting cases

Rayleight scattering elastic scattering

$$|I\rangle = |F\rangle\,, \tag{7.31a}$$

$$\omega_i = \omega_f \tag{7.31b}$$

$$\hbar\omega \ll E_I - E_N \tag{7.31c}$$

combine $\boldsymbol{\epsilon}_i \cdot \boldsymbol{\epsilon}_f$ with other terms

$$
\begin{aligned}
\langle I| \boldsymbol{\epsilon}_i \boldsymbol{\epsilon}^*_f |I\rangle &= \frac{1}{i\hbar} \langle I| \left[\mathbf{x}\cdot\boldsymbol{\epsilon}_i, \mathbf{p}\cdot\boldsymbol{\epsilon}^*_f\right] |I\rangle \\
&= \frac{1}{i\hbar} \sum_N \big(\langle I| \mathbf{x}\cdot\boldsymbol{\epsilon}_i |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}^*_f |I\rangle \\
&\qquad - \langle I| \mathbf{p}\cdot\boldsymbol{\epsilon}^*_f |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}^*_f |I\rangle \big)
\end{aligned} \tag{7.32a}
$$

$\rightarrow$ put everything together:

$$\frac{1}{E_N - E_I} + \frac{1}{E_I - E_N + \pm\hbar\omega} = \mp \frac{\hbar\omega}{\left(E_I - E_N\right)^2} + \frac{\left(\hbar\omega\right)^2}{\left(E_I - E_N\right)^2} + \dots \tag{7.33a}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = r_0^2 \frac{\left(\hbar\omega\right)^4}{m^2} \left| \sum_N \frac{\langle I| \mathbf{p}\cdot\boldsymbol{\epsilon}^*_f |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}_i |I\rangle}{\left(E_I - E_N\right)^2} + \leftrightarrow \right|^2$$

r_0^2 classical e-radius, ω^4 blue sky red sunset

$$\hbar\omega_i \gg E_N - E_I \tag{7.34a}$$

(large compared to bindig energy $\rightsquigarrow$ scattering off "free" electrons)

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = r^2 \left|\boldsymbol{\epsilon}_i \cdot \boldsymbol{\epsilon}_f\right|^2 \tag{7.34b}$$

for unpolarized photons

$$\begin{aligned}
&\frac{1}{2}\sum_{\lambda_i \lambda_f} \varepsilon_i^a \left(k_i, \lambda_i\right) \left(\varepsilon_f\right)^a \left(k_f, \lambda_f\right) \varepsilon_i^b \left(\varepsilon_f^*\right)^b \\
&= \frac{1}{2}\left(\delta_{ab} - \frac{k_i^a k_i^b}{k_i^)}\right)\left(\delta_{ab} - \frac{k_f^a k_f^b}{k_f^2}\right) \\
&= \frac{1}{2}\left(1 + \cos^2\theta\right)
\end{aligned} \tag{7.34c}$$

with

$$\theta = \sphericalangle\left(\mathbf{k}_i, \mathbf{k}_f\right) \tag{7.34d}$$

$$\begin{aligned}
\sigma &= \int \mathrm{d}\cos\theta \, 2\pi r_0^2 \left(1 + \cos^2\theta\right) \\
&= \frac{8\pi}{3} r_0^2
\end{aligned} \tag{7.34e}$$

Resonances What if $E_N \sim E_I + \hbar\omega_i$
so far : neglected finite lifetime of E_N, $\tau_N = \frac{\hbar}{\Gamma_N}$
time evolution

$$e^{-\frac{i}{\hbar}E_N t} e^{-\tau_N t} = e^{-\frac{i}{\hbar}t\left(E_N - i\Gamma_N\right)} \tag{7.35a}$$

with Γ_N that one cannot neglect

$$\begin{aligned}
\left|T\right|^2 &\approx \left|\frac{1}{E_I - E_N + i\Gamma_N}\right|^2 \\
&= \frac{1}{\left(E_I - E_N\right)^2 + \Gamma_N^2}
\end{aligned} \tag{7.35b}$$

Chapter 8

Relativistic QM

Will wry to find relativistic generalization of Schrödinger as single-particle equation ($\rightarrow$ we will fail) but will be basis of relativistic ($2nd$ quantized field theory) Rel: Cannot fix number of particles

8.1 Klein-Gordon equation (KGE)

Consider dfree scalar particle

$$\begin{aligned} X^\mu &\rightarrow X^{\mu'} \\ &= \Lambda^\mu_{\ \nu} x^\nu \end{aligned} \tag{8.1a}$$

$$\begin{aligned} \phi(x) &\rightarrow \phi'(x') \\ &= \phi(x) \\ &= \phi\left(\Lambda^{-1} x'\right) \end{aligned} \tag{8.1b}$$

Now start from

$$E^2 = m^2 c^4 + \mathbf{p}^2 c^2 \tag{8.2a}$$

$(not\ E = \frac{p^2}{2m})$

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \tag{8.2b}$$

$$\mathbf{p} = -i\hbar \boldsymbol{\nabla} \tag{8.2c}$$

$$\left(-\hbar^2 \frac{\partial^2}{\partial t^2}\right) \phi(\mathbf{x}, t) = \left(m^2 c^4 - \hbar c^2 \boldsymbol{\nabla}^2\right) \phi(x, t) \tag{8.2d}$$

in covariant form:

$$\partial_\mu \partial^\mu + \frac{m^2c^2}{\hbar^2}\phi(x) = 0 \tag{8.2e}$$

$$\begin{aligned}\partial_\mu &= \frac{\partial}{\partial x^\mu} \\ &= \left(\frac{1}{c}\frac{\partial}{\partial t}, \boldsymbol{\nabla}\right)\end{aligned} \tag{8.2f}$$

$$\partial^\mu = \left(\frac{1}{c}\frac{\partial}{\partial t} - \boldsymbol{\nabla}\right) \tag{8.2g}$$

8.2 Klein-Gordon equation

KGE:

$$\left(\partial_\mu \partial^\mu + \frac{m^2c^2}{\hbar^2}\right)\phi = 0 \tag{8.3a}$$

$$\partial_\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, \boldsymbol{\nabla}\right) \tag{8.3b}$$

Solution

$$\phi\left(t, \mathbf{x}\right) = A \cdot e^{i\mathbf{k}\cdot\mathbf{x} - i\omega t} \tag{8.3c}$$

$$\phi(x) = A \cdot e^{-ik_\mu x^\mu} \tag{8.3d}$$

$$k^\mu = \left(\frac{\omega}{c}, \mathbf{k}\right), \quad k^2 = k_\mu k^\mu = \frac{\omega^2}{c^2} - \mathbf{k}^2 = \frac{m^2c^2}{\hbar^2} \tag{8.3e}$$

or

$$(h\omega) = \pm\sqrt{m^2c^4 + \mathbf{p}^2c^2} \tag{8.3f}$$

Negative solutions?!

In analogy to Schrödinger, try to define probability density $\rho(\mathbf{x}, t)$ and probability current density $\mathbf{j}\left(\mathbf{x}, t\right)$ satisfying

$$\frac{\partial}{\partial t}\rho + \boldsymbol{\nabla}\mathbf{j} = 0 \tag{8.4a}$$

$$\mathbf{j} = \frac{\hbar}{2mi}\left(\phi^*\left(\nabla\phi\right) - \left(\nabla\phi^*\right)\phi\right) \tag{8.4b}$$

$$\rho = \frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial t} - \frac{\partial\phi^*}{\partial t}\phi\right) \tag{8.4c}$$

covariant form

$$\begin{aligned} j^{\mu} &= (cp, j) \\ &= \frac{i\hbar}{2m}\left(\phi^* \partial^{\mu} \phi - \left(\partial^{\mu} \phi^*\right) \phi\right) \end{aligned} \tag{8.4d}$$

Note that $\rho(\mathbf{x}, t)$ is *not* positive definite $\rightarrow$ cannot be interpreted as probability density

8.3 Dirac equation

Try a linear (in $\frac{\partial}{\partial t}, \boldsymbol{\nabla}$) equation. Mostgeneral linear equation.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \psi &= H\psi \\ &= \left(-i\hbar c \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta m c^2\right) \psi \\ &= \left(-i\hbar c \alpha_i \nabla_i + \beta m c^2\right) \psi \end{aligned} \tag{8.5a}$$

With summation convention and

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3) \tag{8.5b}$$

and β are 4 non-commeting coefficients

Iterate tis equation

$$\begin{aligned} -\hbar^2 \frac{\partial^2}{\partial t^2} \psi &= \left(-i\hbar c \alpha_i \nabla_i + \beta m c^2\right)\left(-i\hbar c \alpha_j \nabla_j + \beta m c^2\right) \psi \\ &= \Bigg(c^2 \frac{\hbar^2}{2} \left(\alpha_i \alpha_j + \alpha_j \alpha_i\right) \nabla_i \nabla_j - i\hbar \left(\alpha_i \beta + \beta \alpha_i\right) \nabla_i m c^2 \\ &\qquad + \beta m^2 c^4 \Bigg) \psi \end{aligned}$$

Compare to KGE

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \psi = \left(-\hbar c^2 \nabla_i \nabla_i + m^2 c^4\right) \psi \tag{8.6a}$$

$$\beta^2 = 1 \tag{8.6b}$$

$$\begin{aligned} \left(\alpha_i \beta + \beta \alpha_i\right) &= \{\alpha_i, \beta\} \\ &= 0, \quad (\text{sometimes } [\alpha_i, \beta]_+) \end{aligned} \tag{8.6c}$$

$$\begin{aligned} \left(\alpha_i \alpha_j + \alpha_j \alpha_i\right) &= \{\alpha_i, \alpha_j\} \\ &= 2\delta_{ij} \end{aligned} \tag{8.6d}$$

From anticommutation relations we see that coeff. cannot be “numbers”. ($\rightarrow$ Exercise dim 4 matrices are simplest possibility)
$\rightarrow$ wave function

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \tag{8.7}$$

and one possible choice for $\boldsymbol{\alpha}$ and β.

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \tag{8.8a}$$

$$\begin{aligned} \beta &= \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \text{Dirac representiation} \end{aligned} \tag{8.8b}$$

Rewrite Dirac equation in terms of γ matrices (4×4 again)

$$\gamma^\mu, \quad \mu \in \{0,1,2,3\}, \gamma^0 = \beta, \gamma^i = \beta\alpha^i \tag{8.9a}$$

in Dirac representation

$$\gamma^0 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \tag{8.9b}$$

$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \tag{8.9c}$$

Note cane use any other representation:

$$\gamma^\mu \rightarrow U\gamma^\mu U^{‘]} \tag{8.10a}$$

Take β: Dirac equation

$$\beta \cdot \left(i\hbar \frac{\partial}{\partial t} \right) \psi = \beta \left(-i\hbar c \alpha_i \nabla_i + \beta mc^2 \right) \psi \tag{8.10b}$$

$$i\hbar \frac{\partial}{\partial t} \gamma^0 \psi = \left(-i\hbar c \gamma^i \nabla_i + mc^2 \right) \psi \tag{8.10c}$$

$$\left(i\hbar \partial_\mu - mc \right) \psi = 0 \tag{8.10d}$$

Notation any 4-vector a^μ:

$$\not{a} \equiv a_\mu \gamma^\mu \tag{8.10e}$$

(ϕ and $\not{\partial}$ have been mistaken…)

$$(i\hbar\, \not{\partial}\, - mc)\, \psi = 0 \tag{8.10f}$$

Properties of γ matrices:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \tag{8.10g}$$

$$\gamma^0 \gamma^\mu \gamma^0 = (\gamma^\mu)^\dagger \tag{8.10h}$$

(There is an old notation in Sakurai.) Dirac equation:

$$\begin{aligned}(i\hbar\partial_\mu\gamma^\mu - mc)\, \psi &\equiv \left(i\hbar\not{\partial} - mc\right) \psi \\ &= 0\end{aligned} \tag{8.11a}$$

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\, \mathrm{Id} \tag{8.11b}$$

The adjoint Dirac equation

$$\begin{aligned}0 &= \gamma^+ \left(i\hbar\partial_\mu \left(\gamma^\mu\right)^\dagger - mc\right) \\ &= \psi^\dagger \left(-i\hbar \overleftarrow{\partial}_\mu \gamma^0\gamma^\mu\gamma^0 - \gamma^0\gamma^0 - \gamma^0\gamma^0 mc\right) \\ &= \psi^\dagger\gamma^0 \left(\overleftarrow{\partial}_\mu - mc\right) \gamma^0 \\ &= 0\end{aligned} \tag{8.11c}$$

$$\Rightarrow \overline{\psi}\left(i\hbar\not{\partial} + mc\right) = 0 \tag{8.11d}$$

$$\overline{\psi} \equiv \psi^\dagger\gamma^0 \tag{8.11e}$$

The current:

$$j^\mu \equiv \overline{\psi}\gamma^\mu\psi \tag{8.12a}$$

$$\begin{aligned}\partial_\mu j^\mu &= \left(\not{\partial}\overline{\psi}\right)\psi + \overline{\psi}\not{\partial}\psi \\ &= 0\end{aligned} \tag{8.12b}$$

$$\begin{aligned}\rho &\equiv j^0 \\ &= \psi^\dagger\gamma^0\gamma^0\psi \\ &= \psi^\dagger\psi, \quad \text{positive definite}\end{aligned} \tag{8.12c}$$

($\rightarrow$ we still will have problem with $E < 0$ solutions)

8.4 Coraviance of Dirac equation

Consider LT

$$\begin{aligned} x^\mu &\to x'^\mu \\ &= \Lambda^\mu{}_\nu x^\nu \\ &= \frac{\partial x'^\mu}{\partial x^\nu} x^\nu, \quad (x \to \Lambda x) \end{aligned} \tag{8.13a}$$

Dirac

$$(i\hbar\partial_\mu\gamma^\mu - mc)\,\psi(x) = 0 \tag{8.13b}$$

$$\to \left(i\hbar\partial'_\mu - mc\right)\psi\left(x'\right) = 0 \tag{8.13c}$$

require transformation

$$\begin{aligned} \psi(x) &\to \psi'(x') \\ &= S\left(\Lambda\right)\psi(x) \end{aligned} \tag{8.13d}$$

such that the "new" equation holds start from $S(\Lambda)\times$Dirac equation

$$\begin{aligned} S(\Lambda)\left(i\hbar\frac{\partial}{\partial x^\mu}\gamma^\mu - mc\right)\psi &= S\left(\Lambda\right)\left(i\hbar\Lambda^\nu{}_\mu\partial'_\nu\gamma^\mu - mc\right)\psi \\ &= S(\Lambda)\left(i\hbar\Lambda^\nu{}_\mu\partial'_\nu\gamma^\mu - mc\right)\psi \\ &= \Big(i\hbar S(\Lambda)\left(\Lambda^\nu{}_\mu\gamma^\mu\right)S^{-1}\left(\Lambda\right)\partial'_\nu \\ &\qquad - mc\Big)\underbrace{S(\Lambda)\psi(x)}_{\psi'(x')} \end{aligned} \tag{8.13e}$$

Compare with Dirac in S'

$$S(\Lambda)\Lambda^\nu{}_\mu\gamma^\mu S^{-1}(\Lambda) = \gamma^\nu \tag{8.13f}$$

or

$$\Lambda^\nu{}_\mu\gamma^\mu = S^{-1}(\Lambda)\gamma^\nu S(\Lambda) \tag{8.13g}$$

A proper LT has 6 parameterns (3rot, 3boos par)

$$\omega_{\rho\sigma} = -\omega_{\sigma\rho}, \quad \text{(antisymmetric)} \tag{8.13h}$$

Claim: For infinitesimal propel LT:

$$S(\Lambda) = \mathbf{1} + \frac{i}{2}\omega_{\mu\nu}\sigma^{\mu\nu} \tag{8.14a}$$

with

$$\sigma^{\mu\nu} \equiv \frac{i}{2}\left[\gamma^\mu, \gamma^\nu\right] \tag{8.14b}$$

or for finite LT

$$S(\Lambda) = e^{\frac{i}{2}\omega_{\mu\nu}\sigma^{\mu\nu}} \tag{8.14c}$$

(compare to QMI rotations) $\rightarrow$ exercise sheet 12

Fro pariti $(t, \mathbf{x}) \rightarrow (t, -\mathbf{x})$ or

$$\Lambda^\mu{}_\nu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{8.15a}$$

we get for $\nu = 0$

$$S\gamma^0 S = \gamma^0 \tag{8.15b}$$

and for $\nu = i$

$$S\gamma^i S = -\gamma^i \tag{8.15c}$$

$$S(\Lambda_p) = \gamma^0 \times \underbrace{\text{Phase}}_{1} \tag{8.15d}$$

Define

$$\gamma_5 \equiv i\gamma_0\psi_1\gamma_2\psi_3 \tag{8.16a}$$

in Dirac representation

$$\gamma_5 = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \tag{8.16b}$$

Note

$$(\gamma_5) = \mathbf{1}\,. \tag{8.16c}$$

Now we can parametrize any 4×4 matrix in terms of the following 16 matrices $\left\{\mathbf{1}, \gamma_5, \gamma^4, \gamma_5\gamma^4, \sigma^{\mu\nu}\right\}$. We know

$$\psi(x) \xrightarrow{\text{LT}} S(\Lambda)\psi(x) \tag{8.17a}$$

$$\overline{\psi}(x) \xrightarrow{\text{LT}} \overline{\psi}(x)S^{-1}(\Lambda) \tag{8.17b}$$

$\rightarrow$ exercise sheet 12

8.4.1 Bilinear covariants

$$\overline{\psi}(x)\psi(x) \xrightarrow{\text{pLT}} \overline{\psi}S^{-1}S\psi = \overline{\psi}(x)\psi(x) \tag{8.18a}$$

$$\xrightarrow{\text{Parity}} \overline{\psi}\gamma^0\gamma^0\psi = \overline{\psi}(x)\psi(x) \tag{8.18b}$$

$$\overline{\psi}(x)\gamma_5(x)\psi(x) \xrightarrow{\text{pLT}} \overline{\psi}S^{-1}\gamma^5 S\psi = \overline{\psi}\gamma_5\psi \tag{8.18c}$$

$$\left\{\gamma^5, \gamma^\mu\right\} = 0 \tag{8.18d}$$

$$\Rightarrow [S, \gamma_5] = 0 \tag{8.18e}$$

$$\overline{\psi}\gamma^\mu\psi \to \Lambda^\mu{}_\nu\overline{\psi}\gamma^\nu\psi, \quad \text{vector} \tag{8.19a}$$

$$\overline{\psi}\gamma_5\gamma^\mu\psi \to \mathrm{Det}(\Lambda)\Lambda^\mu{}_\nu\overline{\psi}\gamma^\nu\gamma_5\psi, \quad \text{axial vector} \tag{8.19b}$$

$$\overline{\psi}\sigma^{\mu\nu}\psi \to \Lambda^\mu{}_\rho\Lambda^\nu{}_\sigma\overline{\psi}\gamma^{\rho\sigma}\psi, \quad \text{tensor rank 2} \tag{8.19c}$$

8.5 Solutions to the dirac equation

$$\psi(x) = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \tag{8.20}$$

4 comps: 2 spin×2 positive/negative energy
momentum space

$$\psi^+(x) = e^{-ikx}u(k), \quad \text{positive } E \tag{8.21a}$$

$$\psi^-(x) = e^{ikx}v(k), \quad \text{negative } E \tag{8.21b}$$

$$\begin{aligned}\mathbf{k}\cdot\mathbf{x} &= k_\mu x^\mu \\ &= \omega t - \mathbf{x}\cdot\mathbf{k}\end{aligned} \tag{8.22a}$$

write as:

$$\psi^+ = e^{-\frac{i}{\hbar}(Et-px)}u(p) \tag{8.22b}$$

$$\psi^- = e^{\frac{i}{\hbar}(-Et-px)}u(p) \tag{8.22c}$$

$$p^\mu = \left(\frac{E}{c}, p\right) \tag{8.22d}$$

Dirac

$$(\not{p} - mc)\, u(p) = 0 \tag{8.23a}$$

$$-\not{p} - mcv(p) = 0 \tag{8.23b}$$

are matrix equations

$$\begin{aligned}(\not{p} \mp mc) &= \begin{pmatrix} \frac{E}{c} \mp mc & -\mathbf{p}\cdot\boldsymbol{\sigma} \\ \mathbf{p}\cdot\boldsymbol{\sigma} & -\frac{E}{c} \mp mc \end{pmatrix} \begin{pmatrix} \chi \\ \varphi \end{pmatrix} \\ &= 0\end{aligned} \tag{8.23c}$$

par. of u and/or v

$$u(p) \equiv \begin{pmatrix} \chi \\ \varphi \end{pmatrix} \tag{8.23d}$$

$$\varphi = \left(\frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{E + mc^2} \right) \chi \tag{8.23e}$$

pick normalization factor $\sqrt{E + mc^2}$

$$u\,(p, r) = \begin{pmatrix} \sqrt{E + mc^2} \quad \chi_r \\ \frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{\sqrt{E+mc^2}} \chi_r \end{pmatrix} \tag{8.23f}$$

and

$$v(p, r) = \begin{pmatrix} \frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{\sqrt{E+mc^2}} & \chi_r \\ \sqrt{E + mc^2} & \chi_r \end{pmatrix} \tag{8.23g}$$

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{8.23h}$$

$$\chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{8.23i}$$

r related to spin, 4-solutions

some propertes of u and v:

$$\overline{u}\,(p, r_i)\, u\,(p, r_j) = u^\dagger\,(p, r_i)\,\gamma^0 u\,(p, R - j) \tag{8.23j}$$

$$\begin{aligned}&\begin{pmatrix} \sqrt{E + mc^2}\chi_i & \frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{\sqrt{E+mc^2}\chi_i} \cdot \end{pmatrix} \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \begin{pmatrix} \sqrt{E + mc^2} & \chi_j \\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{\sqrt{E+mc^2}} & \chi_j \end{pmatrix} \\ &\quad = \left((E + mc^2) \right) \chi_i \cdot \chi_j - \frac{c\mathbf{p}^2}{(Emc^2)} \chi_i \chi_j \\ &\quad = 2mc^2 \chi_i \chi_j \\ &\quad = 2mc^2 \delta_{ij}\end{aligned} \tag{8.23k}$$

similar

$$\overline{v}(p, r_i)\, v(p, r_j) = -2mc^2 \delta_{ij} \tag{8.23l}$$

and

$$\begin{aligned} \overline{v} u &= \overline{u} v \\ &= 0 \end{aligned} \tag{8.23m}$$

Convention: In some books

$$u/v \to \frac{1}{\sqrt{2mc^2}} u/v \tag{8.23n}$$

$\to u, v$ form a basis

We can also show:

$$\sum_{i\,=1}^{3} u(p, r_i) \cdot \overline{u}(p, r_i) = c\,(\not{p} + mc) \tag{8.24a}$$

$\leftarrow$ projection to positios energy states

$$\sum v(p, r_i) \cdot \overline{v}(p, r_i) = c\,(-\not{p} + mc) \tag{8.24b}$$

$\leftarrow$ negative

Show equaivalence for complete set $u(p, r_j)$ and $v(p, r_j)$ e.g.

$$\left(\sum_{i=1}^{3} u(p, r_i) \cdot \overline{u}(p, r_i)\right) u(p, r_j) = 2mc^2 u(p, r_j) \dots \tag{8.24c}$$

8.5.1 Interpretation of solutions and spin

Now we show that Dirac equation describes spin $\frac{1}{2}$

$$H = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc^2 \tag{8.25a}$$

$$\mathbf{L} = \mathbf{x} \times \mathbf{p} \tag{8.25b}$$

$$\begin{aligned} [L_i, H] &= [\varepsilon_{ijk} x_j p_k, \alpha_\ell p_\ell] \\ &= \varepsilon_{ijk} \alpha_\ell [x_j, p_\ell]\, p_k \\ &= i\hbar \varepsilon_{ijk} \alpha_j p_k \end{aligned} \tag{8.25c}$$

$$\begin{aligned} [\mathbf{L}, H] &= i\hbar \boldsymbol{\alpha} \times \mathbf{p} \\ &\neq 0 \end{aligned} \tag{8.25d}$$

is not conserved. However $\mathbf{J} = \mathbf{L} + \mathbf{S}$ must be conserved $\mathbf{S} \neq 0$

need to find $\mathbf{S}$ such that

$$[\mathbf{J}, H] = 0\,, \tag{8.26a}$$

i.e.

$$[\mathbf{S}, H] = -i\hbar\boldsymbol{\alpha} \times \mathbf{p} \tag{8.26b}$$

and of course

$$[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k \tag{8.26c}$$

claim:

$$\begin{aligned} \mathbf{S} &= \frac{\hbar}{2}\sum \\ &= \frac{-i\hbar}{2}\alpha^1\alpha^2\alpha^3\boldsymbol{\alpha} \\ &= \frac{\hbar}{2}\begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \end{aligned} \tag{8.26d}$$

Proof:

$$[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k \tag{8.27a}$$

$$\begin{aligned} [S_i, H] &= \frac{-i\hbar}{2}\left[\alpha^1\alpha^2\alpha^3\alpha^i, H\right] \\ &= \frac{-i\hbar}{2}\frac{1}{2}\left[\alpha^j\alpha^k, \alpha^n p^n + \beta mc^2\right] \end{aligned} \tag{8.27b}$$

with

$$\left[\alpha^j\alpha^k, \beta\right] = 0 \tag{8.27c}$$

use

Let's look at relation between spin and coordinate transformation more carefulle

QMI (nor-rel) [Section 10.4] Translation & rotations: generators P^i, J^i

$$\left[P^i, P^j\right] = 0 \tag{8.28a}$$

$$\left[J^i, J^j\right] = i\hbar\varepsilon^{ijk}J^k \tag{8.28b}$$

$$\left[J^i, P^j\right] = i\hbar\varepsilon^{ijk}P^k \tag{8.28c}$$

coordinate transformation:

$$\begin{aligned}\mathbf{x} &\to \mathbf{x}' \\ &= R\mathbf{x} + \mathbf{a}\end{aligned} \tag{8.28d}$$

a: state $|\psi\rangle$ transformation under a certain representation

$$\begin{aligned}|\psi\rangle &\to |\psi'\rangle \\ &= U(R,a)\,|\psi\rangle\end{aligned} \tag{8.28e}$$

in relativity add boosts

$$x^\mu \to \Lambda^\mu{}_\nu x^\nu + a^\mu \tag{8.28f}$$

$$[K_i, K_j] = -i\hbar\varepsilon_{ijk}J_k \tag{8.28g}$$

$$[K_i, J_i] = i\hbar\varepsilon_{ijk}K_k \tag{8.28h}$$

generator

$$J^{\mu\nu} = \begin{cases} J_{0i} = -J_{i0} = K_i \\ J_{ij} = -J_{ji} = i\varepsilon_{ijk}J_k \end{cases} \tag{8.28i}$$

6 generators $+4$ P^μ

8.5.2 Lie algebra of generators

$$[P_\mu, P_\nu] = 0 \tag{8.29a}$$

$$[J_{\mu\nu}, J_{\rho\sigma}] = i\hbar\left(g_{\nu\rho}J_{\mu\sigma} - g_{\mu\rho}J_{\nu\sigma} - g_{\nu\sigma}J_{\mu\rho} + g_{\mu\sigma}J_{\nu\rho}\right) \tag{8.29b}$$

$$[P_\mu, J_{\rho\sigma}] = i\hbar\left(g_{\mu\rho}P_\sigma - G_{\mu\sigma}P_\rho\right) \tag{8.29c}$$

under Lorentz transform a state $|p,\rangle$ transforms under a certain representation

$$\begin{aligned}|p\rangle &\to |\Lambda p\rangle \\ &= U(\Lambda)\,|p\rangle\end{aligned} \tag{8.29d}$$

$P_\mu P^\mu$ commutes with all generators, P^2 is L-invariant (Casimir). What else do we need to know (Result: “only” transform under rotations, i.e., “spin”)
Consider any P^μ. little group of P^μ:
Subgroup of all Poincaré transformations that leave P^μ invariant
for p^μ in rest frame $p^\mu = (m,0,0,0)$: Little group $\simeq$ rotatinos
Let

$$p^\mu = L^\mu{}_\nu q^\nu \tag{8.30a}$$

i.e. for any q^μ with

$$q^2 = m^2 \\ > 0 \tag{8.30b}$$

we can find LT $L\left(p\right)$, s.t.

$$p = L(p)q \tag{8.30c}$$

is in rest frame ... under any LT, Λ

$$\begin{aligned}\left|p\right\rangle &\to U(\Lambda)\left|p\right\rangle \\ &= U(\Lambda)U\left(L(p)\right)\left|q\right\rangle\end{aligned} \tag{8.30d}$$

$$U\left(L\left(\Lambda p\right)\right)U^{-1}\left(L\left(\Lambda p\right)\right)U(\Lambda)U\left(L(p)\right)\left|q\right\rangle \tag{8.30e}$$

$$U\left(L\left(\Lambda p\right)\right)\cdot U\left(L^{-1}\left(\Lambda p\right)\right)U(\Lambda)U\left(L\left(p\right)\right)\left|q\right\rangle \tag{8.30f}$$

$$U\left(L\left(\Lambda p\right)\right)U\left(L^{-1}\left(\Lambda p\right)\Lambda\cdot L\left(p\right)\right)\left|q\right\rangle \tag{8.30g}$$

$\to$ additional labels in $\left|p, s\right\rangle$ are affected by rotations only

$$\begin{aligned}\left|p, s\right\rangle &\to U(\Lambda)\left|p, s\right\rangle \\ &= U\left(L\left(\Lambda p\right)\right)\underbrace{\sum D_{ss'}}_{\text{def. transformation under rotations}} \\ &= \sum D_{ss'}\left|\Lambda p, s'\right\rangle\end{aligned} \tag{8.31a}$$

8.5.3 2nd casimir operator

$$W_\mu W^\mu = -m^2\hbar^2 s\left(s+1\right) \tag{8.32a}$$

Pauli-Lubanski (axial) vector

$$W_\mu = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}J^{\nu\rho}P^\sigma \tag{8.32b}$$

in rest frame

$$P^\sigma = (m, 0, 0, 0) \tag{8.32c}$$

$$W_\mu = (0, \boldsymbol{\omega}) \tag{8.32d}$$

$$\begin{aligned}W_i &= -\frac{1}{2}\varepsilon_{i\nu\rho\sigma}J^{\nu\rho}P^\sigma \\ &= -\frac{m}{2}\varepsilon_{i\nu\rho\sigma}J^{\nu\rho} \\ &= -mJ_i\end{aligned} \tag{8.32e}$$

8.6 The non-relativistic limit

Consider expansion in $\frac{\mathbf{p}}{m} \sim V$ of Dirac equation.
We will derive the Hamiltionian used in section 2 (for fine structure)
Dirac equation in presence of em field:

$$p^\nu \to p^\nu + \frac{e}{c}A^\nu \tag{8.33a}$$

write

$$\psi = \begin{pmatrix}\chi \\ \eta\end{pmatrix}, \quad \text{2-componenent-spinors} \tag{8.33b}$$

$$\not{p} + \frac{e}{c}\not{A} - mc \tag{8.33c}$$

$$\begin{pmatrix}\chi \\ \eta\end{pmatrix} = \begin{pmatrix} \frac{E}{c} + \frac{e}{c}\phi - mc & -\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma} \\ \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma} & -\left(\frac{E}{c} + \frac{e}{c}\phi + mc\right)\end{pmatrix}\begin{pmatrix}\chi \\ \eta\end{pmatrix} \tag{8.33d}$$
$$= 0$$

$$\Rightarrow \left(\frac{E}{c} + \frac{e}{c}\phi - mc\right)\chi = \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma}\eta \tag{8.33e}$$

$$\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma}\chi = \left(\frac{E}{c} + mc + \frac{e}{c}\phi\right)\eta \tag{8.33f}$$

$$\begin{aligned}\rightsquigarrow \eta &= \frac{\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma}}{\frac{E}{c} + mc + \frac{e}{c}\phi}\chi \\ &\approx \frac{\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\sigma}{2mc}\chi\end{aligned} \tag{8.33g}$$

Putting Eq. 8.33g in Eq. 8.33e gives us

$$\begin{aligned}\left(\frac{E}{c} + \frac{e}{c}\phi - mc\right)\chi &= \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\sigma}\frac{1}{2mc}\chi \\ &= \frac{1}{2mc}\Bigg(\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 \\ &\qquad + i\left(-i\hbar\right)\frac{e}{c}\underbrace{\left(\boldsymbol{\nabla}\times\mathbf{A} + \mathbf{A}\times\boldsymbol{\nabla}\right)}_{[\nabla\times\mathbf{A}]}\cdot\boldsymbol{\sigma}\Bigg)\chi\end{aligned} \tag{8.33h}$$

"derivative within $[\cdot]$ only"

$$\begin{aligned}&\Rightarrow \left(\frac{1}{2m}\left(\mathbf{p}\cdot\frac{e}{c}\mathbf{A}\right)^2+\frac{\hbar e}{2mc}\boldsymbol{\sigma}\cdot\mathbf{B}-e\phi\right)\chi\\ &\quad=\left(E-mc^2\right)\chi\\ &\quad=: E'\chi\end{aligned} \tag{8.33i}$$

where $\frac{\hbar e}{2mc}\boldsymbol{\sigma}\cdot\mathbf{B}$ has to be compare to section 2.3 with

$$\begin{aligned}H &\sim \boldsymbol{\mu}\cdot\mathbf{B}\\ &=\frac{e}{2m}g\mathbf{S}\cdot\mathbf{B}\\ &=\frac{e}{4m}g\boldsymbol{\sigma}\cdot\mathbf{B}\end{aligned} \tag{8.33j}$$

$$\Rightarrow g=2 \tag{8.33k}$$

Let's do this more systematically (expand in $\frac{|e|}{m}$)
Find transformation

$$\psi=e^{-iS}\psi',\quad \text{(Foldy-Wontthuysen transformation)} \tag{8.34a}$$

such thath odd operators are suppressed by $\left(\frac{|p|}{m}\right)^n \rightsquigarrow$ mixes χ and η

$$\sigma := c\boldsymbol{\alpha}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right) \tag{8.34b}$$

$$\begin{aligned}i\hbar\partial_t\psi' &= i\hbar\partial_t e^{iS}\psi\\ &= i\hbar\left[\partial_t e^{iS}\right]\psi+e^{@S}i\hbar\partial_t\psi\\ &= i\hbar\left[\partial_t e^{+iS}\right]e^{-iS}\psi'+e^{iS}He^{-iS}\psi'\\ &=: H'\psi'\end{aligned} \tag{8.34c}$$

$$\begin{aligned}H' &= H+i\left[S,H\right]+\frac{i^2}{2!}\left[S,\left[S,H\right]\right]+\frac{i^3}{3!}\dots\\ &\quad-\hbar\dot{S}-\frac{i\hbar}{2!}\left[S,\dot{S}\right]-\frac{i^2\hbar}{3!}\left[S,\left[S,\dot{S}\right]\right]\dots\end{aligned} \tag{8.34d}$$

Recall

$$H=\beta mc^2+\sigma+\xi,\quad \text{even: } \xi=-e\phi \tag{8.34e}$$

Set

$$S=\frac{-i\beta}{2mc^2}\sigma \tag{8.34f}$$

Compute

$$
\begin{aligned}
i\,[S,H] &= i\left[\frac{-i\beta}{2mc^2}\sigma, \beta mc^2+\sigma+\xi\right] \\
&= \frac{\beta}{2mc^2}\,[\sigma,\xi] + \frac{\beta}{mc^2}\sigma^2 - \sigma
\end{aligned}
\tag{8.34g}
$$

8.7 Observables in 2nd quantization

Observables expressed in terms of fields /*to* operators in Fock space $\mathcal{F}$.
Example: particle number density

QM: probability density

$$\rho(x) = |\psi(x)|^2 \tag{8.35}$$

now:

$$
\begin{aligned}
\hat{\rho(x)} &= \hat{\psi}^\dagger(x)\hat{\psi}(x) \\
&= \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \psi_i^*(x)\psi_j(x) \\
&= \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \langle x|i\rangle \langle j|x\rangle
\end{aligned}
\tag{8.36a}
$$

$$
\begin{aligned}
\int \mathrm{d}^3\mathbf{x}\,\hat{\rho}(x) &= \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \langle j| \underbrace{\int \mathrm{d}^3x\,|x\rangle\langle x|}_{\mathbf{1}} |i\rangle \\
&= \sum_i \hat{a}_i^\dagger \hat{a}_i \\
&= \sum_i n_i
\end{aligned}
\tag{8.36b}
$$

$$\hat{T} = \int \mathrm{d}^3\mathbf{x}\,\hat{\psi}^\dagger \left(-\frac{\hbar^2\nabla^2}{2m}\right)\hat{\psi}(x) \tag{8.37a}$$

$$\hat{\psi}(x) = \sum_i \hat{a}_i \psi_i(x) \tag{8.38a}$$

$$\hat{\psi}^\dagger(x) = \sum_i \hat{a}_i^\dagger \tag{8.38b}$$

$$\hat{\psi}(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \hat{a}_k e^{-i\mathbf{k}\cdot\mathbf{x}} \tag{8.38c}$$

$$\hat{\psi}^\dagger(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \hat{a}_k^\dagger e^{i\mathbf{k}\cdot\mathbf{x}} \tag{8.38d}$$

$$\begin{aligned} \hat{T} &= \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3 k'}{(2\pi)^3} \underbrace{e^{i\mathbf{x}\left(\mathbf{k}-\mathbf{k}'\right)}}_{(2\pi)^3\delta\left(\mathbf{k}-\mathbf{k}'\right)} \hat{a}_k^\dagger \hat{a}_{k'} \left(-\frac{\hbar^2 \left(i\mathbf{k}'\right)^2}{2m}\right) \\ &= \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\hbar^2 \mathbf{k}^2}{2m} \underbrace{\hat{a}_k^\dagger \hat{a}_k}_{N_k} \end{aligned} \tag{8.38e}$$

N_k counts number of particles of kind k. Potential

$$U(x) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{-i\mathbf{q}\cdot\mathbf{x}} \tilde{U}(\mathbf{q}) \tag{8.38f}$$

$$\begin{aligned} \hat{U} &= \int \mathrm{d}^3\mathbf{x}\, \hat{\psi}^\dagger(x) U(x) \hat{\psi}(x) \\ &= \int \frac{\mathrm{d}^3 k_1}{(2\pi)^3} \int \frac{\mathrm{d}^3 \mathbf{k}_2}{(2\pi)^3} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \int \underbrace{\mathrm{d}^3 x\, e^{i\mathbf{k}_1\cdot\mathbf{x}} e^{-i\mathbf{k}_2\cdot\mathbf{x}} e^{-i\mathbf{q}\cdot\mathbf{x}}}_{(2\pi)^3\delta(\mathbf{k}_1-\mathbf{k}_2-\mathbf{q})} \hat{a}_{k_1}^\dagger \hat{a}_{k_2} \tilde{U}(\mathbf{q}) \\ &= \int \frac{\mathrm{d}^3 \mathbf{k}_1}{(2\pi)^3} \int \frac{\mathrm{d}^3 \mathbf{k}_2}{(2\pi)^3} \tilde{U}(\mathbf{k}_1 \mathbf{k}_2) \end{aligned} \tag{8.38g}$$

$$\begin{aligned} V(x_1, x_2) &= V(x_1 - x_2) \\ &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{-i\mathbf{q}(\mathbf{x}_1-\mathbf{x}_2)} \tilde{V}(q) \end{aligned} \tag{8.38h}$$

$$
\begin{aligned}
\hat{V} &= \int \mathrm{d}^3 x_1 \int \mathrm{d}^3 x_2 \, \hat{\psi}^\dagger\left(x_1\right) \hat{\psi}^\dagger(x_2) V\left(x_1 - x_2\right) \hat{\psi}(x_1)\hat{\psi}(x_2) \\
&= \int \prod_{i=1}^{4} \frac{\mathrm{d}k_i}{\left(2\pi\right)^3} \int \frac{\mathrm{d}^3 q}{\left(2\pi\right)^3} \cdot \int \mathrm{d}^3 x_1 \, e^{i\mathbf{x}_1(\mathbf{k}_1 - \mathbf{k}_3 - \mathbf{q})} \\
&\quad \cdot \int \mathrm{d}^3 x_2 \, e^{i\mathbf{x}_2(\mathbf{k}_2 - \mathbf{k}_4 + \mathbf{q})} \hat{a}^\dagger_{k_1} \hat{a}^\dagger_{k_2} \hat{a}_{k_3} \hat{a}_{k_4} \\
&= \int \frac{\mathrm{d}^3 \mathbf{k}_1}{\left(2\pi\right)^3} \int \frac{\mathrm{d}^3 \mathbf{k}_2}{\left(2\pi\right)^3} \int \frac{\mathrm{d}^3 q}{\left(2\pi\right)^3} \, \hat{a}^\dagger_{k_1} \hat{a}^\dagger_{k_2} \hat{a}_{\mathbf{k}_1 - \mathbf{q}} \hat{a}_{\mathbf{k}_2 + \mathbf{q}} \tilde{V}(q)
\end{aligned}
\tag{8.38i}
$$

consider commutation relation between field operators:

$$
\left[\hat{\psi}(x), \hat{\psi}(y)\right]_{\mp} = \int \frac{\mathrm{d}^3 k}{\left(2\pi\right)^3} \int \frac{\mathrm{d}^3 \mathbf{k}'}{\left(2\pi\right)^3} \int \frac{\mathrm{d}^3 \mathbf{k}'}{\left(2\pi\right)^3} \, e^{-i\mathbf{k}\cdot\mathbf{x}} e^{+i\mathbf{k}'\cdot\mathbf{y}} \underbrace{\left[\hat{a}_k, \hat{a}^\dagger_{k'}\right]}_{(2\pi)^3 \delta\left(\mathbf{k} - \mathbf{k}'\right)} \stackrel{!}{=} \delta\left(\mathbf{x} - \mathbf{y}\right)
\tag{8.39a}
$$

with the $\left(2\pi\right)^3$ of $\left(2\pi\right)^3 \delta\left(\mathbf{k} - \mathbf{k}'\right)$ being convection and generalization of

$$
\left[\hat{a}_i, \hat{a}^\dagger_j\right] = \delta_{ij}
\tag{8.39b}
$$

time dependence of field operator: Schrödinger picture → Heisenberg

$$
\underbrace{\hat{\psi}\left(\mathbf{x}, t\right)}_{\text{Heisenberg}} = e^{\frac{i}{\hbar}\hat{H}t} \underbrace{\hat{\psi}(\mathbf{x})}_{\text{SChrödinger}} e^{\frac{-i}{\hbar}\hat{H}t}
\tag{8.40a}
$$

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{\psi}\left(\mathbf{x}, t\right) &= -\left[\hat{H}, \hat{\psi}\left(\mathbf{x}, t\right)\right] \\
&= -\left[\hat{H}, \hat{\psi}(\mathbf{x})\right] \\
&= -e^{\frac{i}{\hbar}\hat{H}t} \left[\hat{H}, \hat{\psi}(x)\right] e^{-\frac{i}{\hbar}\hat{H}t}
\end{aligned}
\tag{8.40b}
$$

take free case

$$
\hat{H} = \hat{T}, \quad \text{bosons}
\tag{8.40c}
$$

$$
\left[\hat{T}, \hat{\psi}(x)\right] = \int \mathrm{d}^3 y \, \frac{\hbar^2}{2m} \left[\nabla_y \psi^\dagger(y) \nabla_y \hat{\psi}(y), \hat{\psi}(x)\right]
\tag{8.40d}
$$

from now on, don't write ∇_y but ∇

$$
\begin{aligned}
\left[\nabla_y \psi^\dagger(y) \nabla_y \hat{\psi}(y), \hat{\psi}(x)\right] &= \nabla \hat{\psi}^\dagger(y) \varsigma \hat{\psi}(y) \hat{\psi}(x) - \hat{\psi}(x) \nabla \hat{\psi}^\dagger(y) \nabla \hat{\psi}(y) \\
&= \nabla \hat{\psi}^\dagger(y) \hat{\psi}(x) \nabla \hat{\psi}(y) - \hat{\psi}(x) \nabla \hat{\psi}^\dagger(y) \nabla \hat{\psi}(y) \\
&= \nabla \Bigg(\left[\hat{\psi}^\dagger(y), \hat{\psi}(x)\right] \\
&\quad + \hat{\psi}(x) \underbrace{\hat{\psi}^\dagger(y) \Bigg) \nabla \hat{\psi}(y) - \hat{\psi}(x) \nabla \hat{\psi}^\dagger(y) \nabla \hat{\psi}(y)}_{=0} \\
&= \int \mathrm{d}^3 y \, \frac{-\hbar^2}{2m} \nabla_y \delta\left(\mathbf{x} - \mathbf{y}\right) \nabla \hat{\psi}(y) \\
&= \frac{\hbar^2}{2m} \nabla_x^2 \hat{\psi}(x)
\end{aligned}
$$

in free case

$$
i\hbar \frac{\partial}{\partial t} \hat{\psi}(x,t) = -\frac{\hbar^2}{2m} \nabla^2 \hat{\psi}\left(x,t\right) + \diamondsuit \tag{8.40e}
$$

$\diamondsuit$ with interations much more complicated $\rightarrow$ QFT

8.8 Quantization of relativistic fields

- Start with Lagrangian density $\mathcal{L}$ for classical field tehory
- Compute conjugate momentum field
- impose equal-time (anti-) commutation relations

Example 1: free scalar field $\Phi(\mathbf{x}, t) = \Phi(x)$

-

$$
\mathcal{L} = \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} \underbrace{\frac{m^2 c^2}{\hbar^2}}_{\equiv m^2} \Phi^2 - \underbrace{V(\Phi)}_{=0} \tag{8.41a}
$$

free field (no interactions). Action:

$$\begin{aligned} S &= \int \mathrm{d}t \int \mathrm{d}^3x\, \mathcal{L} \\ &= \int \mathrm{d}^3 4x\, \mathcal{L}\left(\Phi, \partial_\mu \Phi\right) \end{aligned} \tag{8.41b}$$

$$\delta S = 0 \tag{8.41c}$$

$$\to \frac{\partial \mathcal{L}}{\partial \Phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \Phi\right)} 90 \tag{8.41d}$$

for our $\mathcal{L}$:

$$-m^2\Phi - \partial_\mu \partial^\mu \Phi = 0 \tag{8.41e}$$

Klein-Gordan equation

- Conjugate momentum field

$$\begin{aligned} \pi\left(\mathbf{x}, t\right) &= \frac{\partial \mathcal{L}}{\partial \Phi} \\ &= \dot{\phi}\left(\mathbf{x}, t\right) \end{aligned} \tag{8.42a}$$

Hamiltonian

$$\begin{aligned} H &= \int \mathrm{d}^3\mathbf{x}\, \pi \dot{\Phi} - L \\ &= \int \mathrm{d}^3x \left(\pi\dot{\phi} - \mathcal{L}\right) \\ &= \frac{1}{2}\int \mathrm{d}^3x \left(\pi^2 + \left(\nabla\Phi\right)^2 + m^2\Phi^2\right) \end{aligned} \tag{8.42b}$$

with $\mathcal{L}$ the Lagrangian density

$$\begin{aligned} \int \mathrm{d}^3x\, \mathcal{L} &= L \\ &= \text{Lagriangian} \end{aligned} \tag{8.42c}$$

- now second quantization:

$$\Phi(x) \to \Phi\hat{(x)} \tag{8.43a}$$

and

$$\pi(x) \to \hat{\pi}(x) \tag{8.43b}$$

$$\begin{aligned}\left[\hat{\phi}\left(\mathbf{x},t\right),\hat{\phi}\left(\mathbf{y},t\right)\right] &= \left[\hat{\pi}\left(\mathbf{x},t\right),\hat{\pi}\left(\mathbf{y},t\right)\right] \\ &= 0\end{aligned} \tag{8.43c}$$

impose

$$\left[\hat{\Phi}\left(\mathbf{x},t\right),\hat{\pi}\left(\mathbf{y},t\right)\right] = i\delta\left(\mathbf{x}-\mathbf{y}\right) \tag{8.43d}$$

$$\sim [x_i, p_j] = i\delta_{ij}, \quad (\hbar = 1) \tag{8.43e}$$

spin 0, bosonic field use $[\cdot,\cdot] = [\cdot,\cdot]_-$ and not $\{\cdot,\cdot\} = [\cdot,\cdot]_+$

now as for radiation field

$$\hat{\Phi}\left(\mathbf{x},t\right) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{2\omega_k}\left(\hat{a}_k e^{i\mathbf{kx}-i\omega_k t} + \hat{a}_k^\dagger e^{-i\mathbf{kx}+i\omega_k t}\right) \tag{8.43f}$$

with $\omega_k = \sqrt{\mathbf{k}^2 + m^2}$ this satisfies KGE

$$\begin{aligned}\hat{\pi}\left(\mathbf{x},t\right) &= \dot{\hat{\Phi}}\left(\mathbf{x},t\right) \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{2\omega_k}\left(-i\omega_k\hat{a}_k e^{i\mathbf{kx}-i\omega_k t} + i\omega_k\hat{a}_k^\dagger e^{-i\mathbf{kx}+i\omega_k t}\right)\end{aligned} \tag{8.43g}$$

Note: change in normalization:

$$\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \to \underbrace{\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2\omega_k}}_{\text{Lorentz invariant}} \tag{8.43h}$$