Quantum Mechanics II

lecture notes

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Notes

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FS 2013

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).

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 $\rightarrow$ 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.

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

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

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

let

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

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

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

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 $\left\langle \psi_k^{(0)} \right|$

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

for $k = n$

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

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

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

this is in conflict

$$\langle \psi_n | \psi_n \rangle = 1 \tag{1.7}$$

$\rightarrow$ sort out at the end.

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

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

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

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

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

$$\Rightarrow \left|\psi_n^{(2)}\right\rangle$$

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

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

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

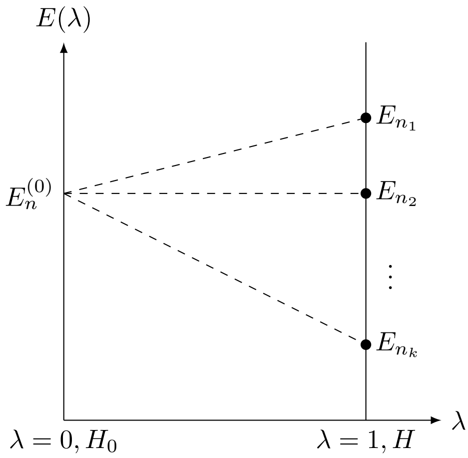

Figure 1.1:

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

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

$\to$ solve

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

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

1.2.1 easy way out (sometimes)

if $V_{ij} = 0$ for $i \neq j$ problem already solved
$\to$ 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 $\left|\psi_{n_i}^{(0)}\right\rangle$ are "good" eigenstates

Proof:

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

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

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

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

Minimize with respect to b

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

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

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

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

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

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

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

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

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

For hydrogen-like atoms

$$V(r) - \frac{Ze^2}{r} \tag{2.7a}$$

QMI uses spherical coordinates

$$\begin{aligned} \psi\left(\mathbf{r}\right) &= R_{E\ell}\left(r\right)\mathcal{Y}_\ell^{m_\ell}\left(\vartheta,\varphi\right) \\ &= \frac{U_{E\ell(r)}}{r}Y_\ell^{m_\ell}\left(\vartheta,\varphi\right) \end{aligned} \tag{2.7b}$$

Then *Schrödinger* $\rightarrow$ differential equation for $U_{E\ell}(r)$

$$U_{E_\ell} - \left(\frac{\ell\left(\ell+1\right)}{r^2} + \frac{2m\left(V(r)-E\right)}{\hbar^2}\right)U_{E\ell} = 0 \tag{2.7c}$$

→ eigenvalues

$$E_n = -\left(\frac{Ze^2}{\hbar}\right)^2 \frac{m}{2n^2}$$
$$= -\frac{(Ze)^2}{2n^2} \tag{2.7d}$$
$$= -\frac{(Ze)^2}{2n^2}\frac{1}{a}$$
$$= -\frac{(Z\alpha)^2}{2n^2}mc^2$$

Bohr radius $a = \frac{\hbar^2}{mc^2}$ (Fine structure constant $\alpha = \frac{\ell^2}{\hbar c} \simeq \frac{1}{137}$)

$$n = 1, 2, 3, \dots \tag{2.7e}$$

$$\ell = 0, 1, \dots, n-1 \tag{2.7f}$$

$$m_\ell = -\ell, -\ell+1, \dots, \ell \tag{2.7g}$$

for each n:

$$2\sum_{\ell=0}^{n-1}(2\ell+1) = 2n^2, \quad \text{degeneracy} \tag{2.7h}$$

where the left-most 2 comes from the electron spin. Eigenfunctions

$$\psi_{n\ell m_\ell} = |n, \ell, m_\ell\rangle$$
$$= \sqrt{\frac{\rho^3\,(n-\ell-1)\,!}{(n+\ell)\,!}} L^{2\ell+1}_{n-\ell+1}(\rho r)e^{-\rho r/2}\,(\rho r)^\ell\,\mathcal{Y}^{m_\ell}_\ell\,(\vartheta, \varphi) \tag{2.7i}$$

2.2 Relativistic corrections

For $Z\alpha \ll 1$: $E_n \ll mc^2$ → non-relativistic system → relativistic corrections are small (so we can use Schrödingers equation)

$$T = \frac{p^2}{2m} \tag{2.8a}$$

$$\to \sqrt{p^2c^2 - m^2c^4} - mc^2 = \frac{p^2}{2m} - \frac{p^4}{8^3c^2} + \dots \tag{2.8b}$$

where $-\frac{p^4}{8m^3c^2}$ are corrections to E_n computed with *perturbation theory*

$$\begin{aligned}
\Delta E_{\text{rel}} &= \langle n,\ell,m_\ell|\,\frac{-p^4}{8m^3c^2}\,|n,\ell,m_\ell\rangle \\
&= -\frac{1}{2mc^2}\,\langle n,\ell,m_\ell|\left(\frac{p^2}{2m}\right)^2|n,\ell,m_\ell\rangle \\
&= -\frac{1}{2mc^2}\,\langle n,\ell,m_\ell|\left(H_0+Z\frac{e^2}{r}\right)^2|n,\ell,m_\ell\rangle \\
&= -\frac{1}{2mc^2}\,\langle n,\ell,m_\ell|\left(H_0+Z\frac{e^2}{r}\right)^2|n,\ell,m_\ell\rangle \\
&= -\frac{1}{2mc^2}\left(E_n^2+2Ze^2E_n\left\langle\frac{1}{r}\right\rangle_{n\ell m_\ell}\right. \\
&\qquad\qquad \left.+\,Z^2e^4\left\langle\frac{1}{r^2}{}_{n\ell m_\ell}\right\rangle\right)
\end{aligned} \tag{2.8c}$$

from exercise

$$\left\langle\frac{1}{r}\right\rangle_{n\ell} = \frac{Z}{an^2}\,, \tag{2.8d}$$

$$\left\langle\frac{1}{r^2}\right\rangle_{n\ell} = \frac{Z^2}{a^2n^3\left(\ell+\frac{1}{2}\right)} \qquad \left\langle\frac{1}{r^3}\right\rangle_{n\ell} = \frac{Z^3}{a^3n^3\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}$$

$$\Delta E_{\text{rel}} = -E_n\underbrace{\frac{\left(Ze^2\right)^2}{\hbar^2c^2}}_{(Z\alpha)^2}\frac{1}{n^2}\left(\frac{3}{4}-\frac{n}{\ell+\frac{1}{2}}\right) \tag{2.8e}$$

2.3 Spin-orbit term

naive "derivation"

(1) Electron with spin → magnetic dipole moment

$$\boldsymbol{\mu} = \frac{e}{m}\frac{g}{2}\mathbf{s}\,, \tag{2.9}$$

$$\mu = \frac{e}{T}\pi r^2\,, \quad s = \frac{2\pi}{T}mr^2\,, \quad g \simeq \text{ (from Dirac)} \tag{2.10}$$

(2) Electron feeds magnetic field due to the proton

$$\mathbf{E} \sim \frac{e}{r3}\mathbf{r} \tag{2.11}$$

$$\begin{aligned} \rightarrow \mathbf{B} &= -\frac{1}{c^2}\boldsymbol{\nabla} \times \mathbf{E} \\ &= -\frac{1}{mc^2 r^3}\mathbf{p} \times \mathbf{r} \\ &= \frac{-\mathbf{L}}{mc^2 r^3} \end{aligned} \tag{2.12}$$

wrong by factor 2 (Thomas precession)

correct result

$$H_{\text{SO}} = \frac{Ze^2}{2mc^2}\frac{1}{r^3}\mathbf{L}\cdot\mathbf{S}, \quad (\sim -\boldsymbol{\mu}\cdot\mathbf{B}) \tag{2.13}$$

To describe spin

$$\begin{aligned} \left| n, \ell, \left(s = \frac{1}{2}, m_s\right)\right\rangle &= \psi_{n\ell m_\ell m_s} \\ &= \psi_{n\ell m_\ell}(r, \theta\varphi)\,\chi_{m_s} \end{aligned} \tag{2.14a}$$

with χ_{m_s} spin-orbit

$$\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \tag{2.14b}$$

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

$$\langle n, \ell, m'_\ell, m'_s|\, H_{\text{SO}}\, |n, \ell, m'_\ell, m'_s\rangle \rightarrow \text{diagonalize} \tag{2.15}$$

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

$$J \equiv L + S \tag{2.16}$$

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

$$|n, \ell, j, m_j\rangle \tag{2.17}$$

$$|n,\ell,j,m_j\rangle = \sum_{m_\ell,m_s} |n,\ell,m_\ell,m_s\rangle \underbrace{\langle n,\ell,m_\ell,m_s|n,\ell,j,m_j\rangle}_{\text{Clebsch-Gordan}} \tag{2.18}$$

use

$$J^2 = L^2 + 2L\cdot S + S^2 \tag{2.19a}$$

$$L\cdot S = \frac{1}{2}\left(J^2 - L^2 - S^2\right) \tag{2.19b}$$

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

$$H_0, L^2, S^2, J^2, J_z \tag{2.20}$$

with eigenvalues

$$E_n, \hbar^2\ell\left(\ell+1\right), \hbar^2\frac{3}{4}, \hbar^2 j\left(j+1\right), \hbar m_j \tag{2.21}$$

$$\Delta E_{\text{SO}} = \langle n,\ell,j,m_j|\, H_{\text{SO}}\, |n,\ell,j,m_j\rangle \tag{2.22}$$

for $\ell = 0$

$$\Delta E_{\text{SO}} = 0 \tag{2.23a}$$

for $\ell \neq 0$

$$\begin{aligned}\Delta E_{\text{SO}} &= \frac{Ze^2}{2m^2c^2}\langle n,\ell,j,m_j|\,\frac{1}{r^3}\frac{1}{2}\left(J^2-L^2-S^2\right)|n,\ell,j,m_j\rangle \\ &= \frac{Ze^2}{2m^2c^2}\left\langle\frac{1}{r^3}\right\rangle\frac{\hbar^2}{2}\left(j\left(j+1\right)-\ell\left(\ell+1\right)-\frac{3}{4}\right) \\ &= -E_n\frac{\left(Z\alpha\right)^2}{2n\left(\ell+\frac{1}{2}\right)}\begin{cases}\frac{1}{\ell+1} & j=\ell+\frac{1}{2}\\ -\frac{1}{\ell} & j=\ell-\frac{1}{2}\end{cases}\end{aligned} \tag{2.23b}$$

2.4 Darwin term

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

$$\langle V\left(r+\delta r\right)\rangle = \langle V(r)\rangle + \underbrace{\frac{1}{2}\langle\boldsymbol{\delta}\rangle\, r\cdot\boldsymbol{\nabla}\boldsymbol{\delta} r\cdot\nabla V} \tag{2.24}$$

correct result is

$$\begin{aligned} H_D &= \frac{\hbar^2}{8m^2c^2}\nabla^2 V \\ &= \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\delta(r) \end{aligned} \tag{2.25}$$

only for $\ell = 0$!

$$\begin{aligned} \Delta E_D &= \langle n,\ell,j,m_j|\, H_D \,|n,\ell,j,m_j\rangle \\ &= \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\,\|\psi_{n\ell}(0)\|^2 \\ &= -E_n\frac{(Z\alpha)^2}{n}\delta_{\ell 0} \end{aligned} \tag{2.26}$$

2.5 Fine structure of hydrogen

Combine ΔE_{rel}, ΔE_{SO} and ΔE_D

$$\Delta E_n = -E_n^{(0)}\frac{(Z\alpha)^2}{n^2}\left(\frac{3}{4} - \frac{n}{j+\frac{1}{2}}\right) \tag{2.27}$$

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

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

2.5.1 first few states

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

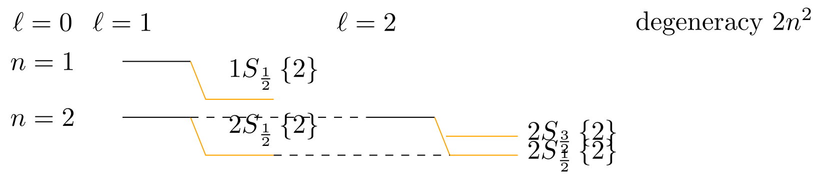

Figure 2.1:

2.6 Corrections beyound fine structure

2.6.1 Hyperfine structure

Effect of proton spin Sp

$$\boldsymbol{\mu}_p = \frac{e}{2m_p} g_p \mathbf{s}_p \tag{2.28}$$

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

$$\rightsquigarrow \Delta E_{\text{Hfs}} \sim (Z\alpha)^4 \frac{m_e}{m_p}\,, \tag{2.29}$$

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

$$\begin{aligned} F &= S_e + S_p \\ &= \begin{cases} 1 & \text{triplet} \\ 0 & \text{singlet} \end{cases} \end{aligned} \tag{2.30}$$

2.6.2 Lamb shift (needs QED!)

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

$$\Delta E_{\text{Lamb}} \sim (Z\alpha)^4 \cdot \alpha \left(\frac{1}{\log (Z\alpha)} \right) \dots \tag{2.31}$$

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:

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

3.1 Identical particles

Consider N identical particles $H(1, .., N)$ wave function $\psi(1, \cdots, N)$.
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

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

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

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

[1]interaction between electrons

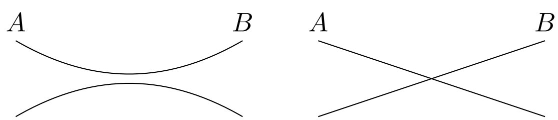

Figure 3.1:

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

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

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

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) totally antisymmetric $|\psi\rangle_A$ with

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

Example $N = 3$

$$\begin{aligned} |\psi\rangle_S = \frac{1}{\sqrt{3!}} \big(&\psi(1,2,3) + \psi(2,1,3) + \psi(1,3,2) + \psi(2,3,1) \\ &+ \psi(3,1,2) + \psi(3,2,1)\big) \end{aligned} \tag{3.9a}$$

$$\begin{aligned} |\psi\rangle_A = \frac{1}{\sqrt{3!}} \big(&\psi(1,2,3) + \psi(2,3,1) + \psi(3,2,1) - \psi(2,1,3) \\ &- \psi(3,2,1) - \psi(1,3,2)\big) \end{aligned} \tag{3.9b}$$

spin-statistics theorem particles with *integer spin* (bosons) are described by *symmetric* wave-functions
particles with *half-integer spin* (fermions) are described by *antisymmetric* wave functions

Bosonic case:

$$\psi_S\left(1,\ldots,N\right) = \frac{1}{\sqrt{N!}} \sum_{p \in S_n} \psi_1\left(P(1)\right) \ldots \psi_N\left(P(N)\right) \tag{3.10a}$$

fermionic case

$$\psi_A\left(1,\ldots,N\right) = \frac{1}{\sqrt{N!}} \sum_{p \in S_n} \left(-1\right)^P \psi_1\left(P(1)\right) \ldots \psi_N\left(P(N)\right) \tag{3.10b}$$

ψ_A can be written as a Slater determinant

$$\psi_A\left(1,\ldots,N\right) = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \psi_1(1) & \cdots & \psi_1(N) \\ \vdots & \ddots & \vdots \\ \psi_N(1) & \cdots & \psi_N(N) \end{pmatrix} \tag{3.10c}$$

Pauli exclusion principle Two identical fermions (same quantum number, s,…) cannot be at the same position. Wave function vanishes for $r_i, r_j; s_i = s_j, \cdots$. i.e. $1 = 2 \rightarrow$ Fermi gas.

3.2 Thomas-Fermi approximation

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

$$V = -\frac{Ze^2}{r} \xrightarrow{\text{other electron}} -e\Phi(r) \tag{3.11}$$

Poisson equation:

$$\boldsymbol{\nabla}^2\Phi = -4\pi\tilde{\rho} \overset{r \geq 0}{=} 4\pi e\rho(r) \tag{3.12}$$

total charge density (other electron and nucleus)

$$\tilde{\rho} = -e\rho(r) + Ze\delta(r) \tag{3.13}$$

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

$$n = \frac{2}{(2\pi\hbar)^3}, \quad \text{if } E = \frac{p^2}{2m} - e\Phi < 0 \tag{3.14a}$$

$$n = 0, \quad \text{if } E = \frac{p^2}{2m} - e\Phi > 0 \tag{3.14b}$$

$$\begin{aligned}\rho &= \int_0^{\sqrt{2me\Phi}} \mathrm{d}^3\, pn \\ &= \frac{(4\pi)\,2}{(2\pi\hbar)^3} \int_0^{\sqrt{2me\phi}} \mathrm{d}p\, p^2 \\ &= \frac{\rho\pi}{3\,(2\pi\hbar)^3}\,(2me\phi)^{3/2}\end{aligned} \tag{3.14c}$$

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

$$\begin{aligned}\boldsymbol{\nabla}^2\Phi &= \frac{1}{R}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Phi(r) \\ &= \frac{32\pi^2 e}{3\,(2\pi\hbar)^3}\,(2me\Phi)^{3/2}\end{aligned} \tag{3.15}$$

solve numerically. boundary condition:

$$\phi(r) \rightarrow \frac{Ze}{r}, \quad \text{for } r \rightarrow 0 \tag{3.16a}$$

normalize

$$4\pi \int \mathrm{d}r\, \rho(r) r^2 = Z \tag{3.16b}$$

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

$$\overline{R} \simeq \text{constant} \cdot a \cdot Z^{1/3} \tag{3.17}$$

3.3 The Hartree approximation

Assume

$$\psi\,(1 \ldots N) = \varphi_1(1) \ldots \varphi_N(N) \tag{3.18a}$$

as solution to

$$H\psi = E\psi \tag{3.18b}$$

with

$$H = \sum_i \left(\frac{p_i^2}{2m} - \frac{Ze^2}{r_i} \right) + \sum_{i>j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{3.18c}$$

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

$$\int \mathrm{d}^3 r_i \, |\varphi_i(r_i)|^2 = 1 \tag{3.19}$$

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

$$\begin{aligned} \langle H \rangle = &\sum_i \int \mathrm{d}^3\mathbf{r} \left(\varphi_i^*(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 - \frac{Ze^2}{r} \right) \varphi_i(r) \right) \\ &+ \sum_{i>j} \int \mathrm{d}^3\mathbf{r} \int \mathrm{d}^3\mathbf{r} \, \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \varphi_i(r) \varphi_j(r') \\ &+ \sum_i \varepsilon_i \left(\int \mathrm{d}^3 r \, |\varphi_i(r)|^2 - 1 \right) \end{aligned} \tag{3.20}$$

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

$$\left(-\frac{\hbar}{2m} \nabla^2 - \frac{Ze^2}{r} \right) \varphi_i + V_i(r) \varphi_i(r) = \varepsilon_i \varphi_i(r) \tag{3.21a}$$

$$V_i(r) = \sum_{j \neq i} \int \mathrm{d}^3 r' \, \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \, |\varphi_j(\mathbf{r}')|^2 \tag{3.21b}$$

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. 3.21b $\rightsquigarrow$ $V_i^{(0)}$ $\rightsquigarrow$ into Eq. 3.21a solve $\rightsquigarrow$ $\varphi_i^{(1)}$ $\rightsquigarrow$ etc.

physical interpretation of Lagrange multipliers ε_i $\varphi_i^* \cdot 3.21a$

$$\Rightarrow \int \mathrm{d}^3 r \left(\frac{-\hbar^2}{2m} \, |\nabla_i \varphi_i|^2 + \left(-\frac{Ze^2}{r_i} + V_i \right) |\varphi_i|^2 \right) = \varepsilon_i \tag{3.22a}$$

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

3.4 Hartree-Fock approximation

improved ansatz for

$$\psi\left(1,\ldots,N\right)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\varphi_1(1) & \cdots & \varphi_N(1)\\ \vdots & \ddots & \vdots\\ \varphi_1(N) & \cdots & \varphi_N(N)\end{vmatrix} \tag{3.23a}$$

fully comptible with Pauli $\rightsquigarrow$ as for Hartree, plug into H and minimize. Eq. 3.21a stayse the same. Eq. 3.21b

$$\begin{aligned}&\frac{1}{2}\sum_{j\neq i}\int \mathrm{d}^3\mathbf{r}_i\int \mathrm{d}^3\mathbf{r}_j\,\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}\\ &\quad\times\big(\varphi_i^*(r_i)\varphi_j^*(r_j)\varphi_i(r_i)\varphi_j(r_j)-\varphi_i^*(r_i)\varphi_j^*(r_j)\varphi_i(r_j)\varphi_j(r_i)\big)\end{aligned} \tag{3.24a}$$

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 $N=2$

$$\psi\left(1,2\right)=\frac{1}{\sqrt{2!}}\left(\varphi_i(1)\varphi_2(2)-\varphi_1(2)\varphi_2(1)\right) \tag{3.25a}$$

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

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

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.

$$\psi_i=R_{n\ell}(r)Y_\ell^m\left(\theta,\varphi\right)\chi_{m_s}\,, \tag{3.26a}$$

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

general rules

$$\begin{cases} n \text{ small} & \text{stronger binding} \\ \ell \text{ small} & \text{electron is closer to nucleus} \end{cases} \tag{3.27}$$

"compete sometimes". for each n :

$$\begin{array}{lcccc} \ell & 0 & 1 & 2 & 3 \\ \text{name} & S & P & D & F \\ \deg 2\,(2\ell+1) & 2 & 4 & 6 & 10 \end{array} \tag{3.28a}$$

$$\begin{array}{lllccc} K\text{-shell} & n=1 & \ell=0 & 2 \text{ elements} & H, He & (1s) \\ L\text{-shell} & n=2 & \ell=0 & 2 & Li, Be & (2s) \\ & & \ell=1 & 6 & B-Ne & (2s) \\ M\text{-shell} & n=3 & \ell=0 & 2 & Na-Mg & (3s) \\ & & \ell=1 & 6 & Al-Ar & (3s) \\ & & \ell=2 & \dots & \dots & (3p) \\ N\text{-shell} & n=4 & \ell=0 & 2 & & (4s) \\ & n=3 & \ell=2 & 10 & Al-Ar & (3d) \\ & n=4 & \ell=1 & 6 & \dots & (4p) \end{array} \tag{3.28b}$$

configuration of electron → chemical properties of elements. What is the configuration (total spin, L, J) ofthe outer electron. → 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 $m_\ell = -1, 0, 1$, $m_s = -\frac{1}{2}, \frac{1}{2}$. → 6 possibilities
for both

$$\frac{6 \cdot 5}{2} = 15 \text{ possibilities} \tag{3.29}$$

$$L = \begin{array}{c} 0,2 \quad \text{symmetric} \\ 1 \;\; \text{anti-symmetric} \end{array} \tag{3.30a}$$

$$S = \begin{array}{c} 1 \quad \text{symmetric} \\ 0 \text{anti-symmetric} \end{array} \tag{3.30b}$$

total wave function is antisymmetric

$$\begin{array}{ccccc} L & S & J & ^{2s+1}L_J & \text{deg} \\ \hline 0 & 0 & 0 & ^1S_0 & 1 \\ & & 0 & ^3P_0 & 1 \\ 1 & 1 & 1 & ^3P_1 & 3 \\ & & 2 & ^3P_2 & 5 \\ 2 & 0 & 2 & ^1D_2 & 5 \\ & & & & 15 \end{array} \tag{3.31}$$

Which one is ground state? → Hund's rules

(1) make spin maximal

$$\begin{aligned} &\to \text{spin part more symmetric} \\ &\to \text{orbital port more asymmetric} \\ &\to \text{electron further away from each other} \\ &\to \text{less repulsion} \end{aligned} \tag{3.32}$$

for C: $s = 1$

(2) make L maximal

$$\begin{aligned} &\to \text{electron average further away from each other} \\ &\to \text{less repulsion} \end{aligned} \tag{3.33}$$

no impaft for C

(3)

$$\Delta E_{\text{SO}} = \text{constant}\,(j\,(j+1) - \ell\,(\ell+1) - s\,(s+1)) \tag{3.34a}$$

$$\text{constant}\begin{cases} > 0 & \text{if subshell } \textit{no} \text{ more than half filled } J = |L - S| \\ < 0 & \text{if subshell more than half filled } J = |L + S| \end{cases} \tag{3.34b}$$

for C first case and

$$\begin{aligned} J &= |L - S| \\ &= 0 \end{aligned} \tag{3.35}$$

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 $\rightarrow$ 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

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

$\to$ into Schrödinger

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

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 ($\to$ 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

$$c_m^{(0)} = \delta_{im} \tag{4.3r}$$

$$\dot{c}_f^{(1)} = (i\hbar)^{-1} V_{fi} e^{i\omega_{fi} t} \tag{4.3s}$$

$$c_f^{(1)}(t) = (i\hbar)^{-1} \int_{t_0}^{t} \mathrm{d}t' V_{fi}(t') e^{i\omega_{fi} t'} \tag{4.3t}$$

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

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

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

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

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

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

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

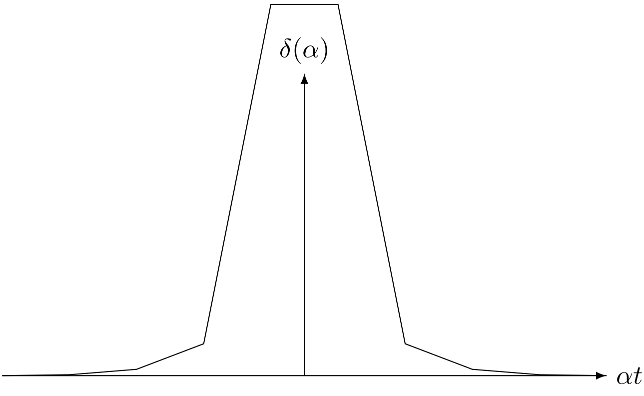

Figure 4.1:

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

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

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

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

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

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

$$= \text{absorption of } \hbar\omega + \text{emission of } \hbar\omega$$

$\rightarrow$ inteaction of matter with radiation

4.4 The Interaction picture

Consider again evolution operator

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

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

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

iii)

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

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

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

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

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

(last step see exercise)

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

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

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.*

T: time ordering

$$T\left(H\left(t_1\right), H(t_2)\right) \equiv H\left(t_1\right) H(t_2)\vartheta\left(t_1 - t_2\right) + H\left(t_2\right) H\left(t_1\right)\vartheta\left(t_2 - t_1\right) \tag{4.12a}$$

$$\begin{aligned} T\left(H\left(t_1\right), H(t_2)H(_3)\right) = & H\left(t_1\right) H\left(t_2\right) H(t_3)\vartheta\left(t_1 - t_2\right)\vartheta\left(t_2 - t_3\right) \\ & + H\left(t_1\right) H\left(t_3\right) H\left(t_2\right)\vartheta\left(t_1 - t_3\right)\vartheta\left(t_3 - t_1\right) \\ & + 4 \text{ more terms} \end{aligned} \tag{4.12b}$$

to make approximations posible, us *interaction picture.* recall

Schrödinger picture:

$$\left|\psi_S(t)\right\rangle, \quad A_S \text{ (time independent)} \tag{4.13}$$

with $\psi_S(t)$ time dependent

Heisenberg picture:

$$\begin{aligned} \left|\psi\right\rangle_H &= \left|\psi(t_0)\right\rangle \\ &= U\left(t_0, t\right)\left|\psi(t)\right\rangle \end{aligned} \tag{4.14a}$$

with

$$A_H(t) = U\left(t_0, t\right) A U\left(t, t_0\right) \tag{4.14b}$$

interaction picture:

$$H = H_0 + V(t) \tag{4.15a}$$

with H_0 time independent

$$U_0\left(t,t_0\right) = e^{-\frac{i}{\hbar}H_0(t-t_0)} \tag{4.15b}$$

$$\begin{aligned}\psi\left(t\right)_I =& \\ &\equiv U_0\left(t_0,t\right)\left|\psi(t)\right\rangle \\ &= U_0\left(t_0,t\right)U\left(t,t_0\right)\left|\psi\right\rangle_H\end{aligned} \tag{4.15c}$$

$$A_I(t) \equiv U_0\left(t_0,t\right)AU_0\left(t,t_0\right) \tag{4.15d}$$

$A_I(t)$ and $|\psi(t)\rangle$ both time dependent

Time evolution in interaction picture

$$\left|\psi(t)\right\rangle_I = U_I\left(t,t_1\right)\left|\psi(t_1)\right\rangle_I \tag{4.16a}$$

where

$$U_I\left(t,t_1\right) = U_0\left(t_0,t\right)U\left(t,t_1\right)U_0\left(t_1,t_0\right) \tag{4.16b}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}U_I\left(t,t_1\right) = V_I(t)U_I\left(t,t_1\right)} \tag{4.17}$$

$$i\hbar\frac{\partial}{\partial t}U\left(t,t_1\right) = H(t)U\left(t,t_1\right) \tag{4.18}$$

$$\boxed{U_I\left(t,t_1\right) = Te^{-\frac{i}{\hbar}\int_{t_1}^{t}\mathrm{d}t'\,V_I(t')}} \tag{4.19}$$

If $V(t)$ "small", can do perturbation theory by expanding exponential. Structure of expansion

$$U_I\left(t,t_0\right) = 1 + (i\hbar)^{-1}\int_{t_0}^{t}\mathrm{d}t\,V_I(t) + (i\hbar)^{-1}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t_1}\mathrm{d}t_2\,V_I(t_1)V_I(t_2) + \dots \tag{4.20}$$

Compurae to Chapter 4.1. Let $V(t) = 0$ for $t < t_0$

Amplitude for initial state $\left|\psi_i^{(0)}\right\rangle$ to go over into final state

$$\begin{aligned}\left\langle\psi_f^{(0)}\middle|\psi_i(t)\right\rangle &= \left\langle\psi_f^{(0)}\middle|U_I(t,t_0)\middle|\psi_i^{(0)}\right\rangle \\ &= \underbrace{\left\langle\psi_f^{(0)}\middle|\psi_i^{(0)}\right\rangle}_{\delta_{if}} + (i\hbar)^{-1}\left\langle\psi_f^{(0)}\middle|\int_{t_0}^{t}\mathrm{d}t'\,V_I(t')\middle|\psi_i^{(0)}\right\rangle\end{aligned} \tag{4.21a}$$

where

$$\left\langle\psi_f^{(0)}\right|\int_{t_0}^{t}\mathrm{d}t'\,V_I(t')\left|\psi_i^{(0)}\right\rangle = \int_{t_0}^{t}\mathrm{d}t'\,\left\langle\psi_f^{(0)}\right| e^{-\frac{i}{\hbar}\left(t_0-t'\right)}V(t')e^{-\frac{i}{\hbar}H\left(t'-t_0\right)}\left|\psi_i^{(0)}\right\rangle$$
$$= \int_{t_0}^{t}\mathrm{d}t'\,\left\langle\psi_f^{(0)}\right| V(t')e^{\frac{i}{\hbar}(E_F-E_i)t'}\left|\psi_i^{(0)}\right\rangle \tag{4.21b}$$

4.5 The adiabatic approximation

Here $V(t)$ *not* small by change is slow

Theorem 4.5.1: For an adiabatic change $H_i \to H_F$ a system that is initialy i nthe nth eigenstate of H_i will evolve into the nth eigenstate of H_f (no level crossing).

Proof: Let

$$H(t) = E_n\,(t)\,|\psi_n(t)\rangle \tag{4.22a}$$

$$|\psi(t)\rangle = \sum_n c_n(t)e^{(i\hbar)^{-1}\int_0^t \mathrm{d}\tau\, E_n(\tau)}\,|\psi_n(t)\rangle$$
$$= \sum_n c_n e^{iE_n}\,|\psi_n(t)\rangle \tag{4.22b}$$

to into Schrödinger

$$i\hbar\sum_n\left(C_n^i\,|\psi_n\rangle + c_n\left|\dot{\psi_n}\right\rangle\right)e^{iE_n} = \sum_n c_n e^{iE_n}H\,|\psi_n\rangle \tag{4.23a}$$

multiply by $\langle\psi_m|$

$$\dot{c}_m = -\sum c_n\,\langle\psi_m|\,\dot{\psi}_n\rangle\,e^{i(E_n-E_m)} \tag{4.23b}$$

where we need to compute $\langle\psi_m|\,\dot{\psi}_n\rangle$

$$H\,|\psi_n\rangle =_n |\psi_n\rangle \tag{4.24a}$$

$$\dot{H}\,|\psi_m\rangle + H\left|\dot{\psi}_n\right\rangle = \dot{E}_n\,|\psi_n\rangle + E_n\left|\dot{\psi}_n\right\rangle \tag{4.24b}$$

$m \not n$

$$\langle\psi_m|\,\dot{H}\,|\psi_n\rangle = (E_n - E_m)\,\langle\psi_m|\,\dot{\psi}_n\rangle \tag{4.24c}$$

into equation for $\dot{c}_m$

$$\dot{c}_m = -c_m\,\langle\psi_m|\,\dot{\psi}_m\rangle - \sum_{n\neq m} c_n \frac{\langle\psi_m|\,\dot{H}\,|\psi_n\rangle}{(E_n - E_m)} \tag{4.24d}$$

adiabatic approximation $\dot{H}$ small $\to 0$ also must not have degeneracy

$$\dot{c}_m(t) = -c_m\,\langle\psi_m|\,\dot{\psi}_m\rangle \tag{4.25a}$$

$$\to c_m(t) = c_m(t_0)e^{i\gamma_m(t)} \tag{4.25b}$$

$$\gamma_m(t) = i\int_{t_0}^{t} \mathrm{d}\tau\;\langle\psi_m(\tau)|\,\dot{\psi}_m(\tau)\rangle \tag{4.25c}$$

if system is in state $|\psi_m\rangle$ at time t it remains in this state

$$\begin{aligned}\psi(t) &= c_m(t)e^{iE_m(t)}\,|\psi_m(t)\rangle \\ &= e^{i\gamma_m(t)}e^{iE_m(t)}\,|\psi_m(t)\rangle\end{aligned} \tag{4.25d}$$

where $e^{i\gamma_m(t)}$ is the geometric phase ($\to$ Berry phase) and $e^{iE_m(t)}$ is the dynamic phase

Chapter 5

Interaction of matter with classical radiation

Here radiation treated as a classical field (quantization of radiation → Chaptor 8)

5.1 Basics from EM & QMI

External classicial field

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} \tag{5.1a}$$

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \dot{\mathbf{A}} \tag{5.1b}$$

(in relativity ϕ, $A \to A^\mu$ not here)
physics invariant und er gauge transformation

$$A^\mu \to A^\mu + \partial^\mu \chi \begin{cases} \mathbf{A} \to \mathbf{A} + \boldsymbol{\nabla}\chi\left(\mathbf{r}, t\right) \\ \phi \to \phi - \frac{1}{c}\dot{\chi}\left(\mathbf{r}, t\right) \end{cases} \tag{5.2a}$$

gauge choice: here *Coulomb gauge*

$$\boldsymbol{\nabla} \cdot \mathbf{A} = 0 \tag{5.3a}$$

Maxwell equation in free space → wave equation for $\mathbf{A}$

$$\begin{aligned} \Box\mathbf{A} &= \left(\frac{1}{c)}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\mathbf{A} \\ &= 0 \end{aligned} \tag{5.3b}$$

solution

$$\begin{aligned} \mathbf{A} = \int \frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3} \sum_\lambda &\left(\chi\left(k,\lambda\right)\boldsymbol{\epsilon}\left(k,\lambda\right)e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_k t}\right. \\ &\left. + \alpha^*\left(\mathbf{k},\lambda\right)\epsilon^*\left(\mathbf{k},\lambda\right)\boldsymbol{\epsilon}^*\left(\mathbf{k},\lambda\right)e^{-i\mathbf{k}\cdot\mathbf{r}} + i\omega_k t\right), \end{aligned} \tag{5.3c}$$

where $\alpha(\mathbf{k},\lambda)$ is the coefficient of linear combination and λ is the polarization $\lambda \in \{1,2\}$ and $\mathbf{k}\cdot\boldsymbol{\epsilon} = 0 \rightarrow 2$ polarizations from $\Box A = 0$ ($\rightarrow \omega_k = c\,|\mathbf{k}|$).

Recall QMI Chapter 9

$$\begin{aligned} H &= \frac{1}{2m}\left(i\hbar\boldsymbol{\nabla} - \frac{q}{c}\mathbf{A}\right)^2 + q\phi + V_0 \\ &= \underbrace{\frac{p^2}{2m} + V_0}_{H_0} - \underbrace{\frac{q}{2mc}\left(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}\right) + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi}_{V(t)} \end{aligned} \tag{5.4a}$$

Introduce *number density:*

$$\begin{aligned} \rho(\mathbf{r}) &= \sum_i \delta\left(\mathbf{r} - \mathbf{r}_i\right) \\ &= \delta\left(\mathbf{r} - \mathbf{r}_1\right) \end{aligned} \tag{5.5}$$

and *current density:*

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2m}\sum_i \left(\mathbf{p}_i\delta\left(\mathbf{r} - \mathbf{r}_i\right) + \delta\left(\mathbf{r} - \mathbf{r}_i\right)\mathbf{p}_i\right) \tag{5.6}$$

then rewrite

$$V(t) = \int \mathrm{d}^3 r\,\left(\frac{e}{c}\mathbf{j}(\mathbf{r})\mathbf{A}\left(\mathbf{r},t\right) + \frac{e^2}{2mc^2}\rho(\mathbf{r})\mathbf{A}^2 - e\rho(\mathbf{r})\phi\left(\mathbf{r},t\right)\right) \tag{5.7a}$$

where $\mathbf{j}(\mathbf{r})$ is the dominant term, $\rho(\mathbf{r})$ drop $\sim \frac{e^2}{c^2}$ (small compared to $\mathbf{j}\cdot\mathbf{A}$) and $\phi(\mathbf{r},t), \phi = 0$. Write $V\left(\mathbf{r}_1, t\right)$ for a single electron in terms of Fourier transform

$$\begin{aligned} \mathbf{j}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{j}(\mathbf{r}) \\ &= \left(\frac{\mathbf{p}_1}{2m}e^{-ik\mathbf{r}_1} + e^{-i\mathbf{k}\mathbf{r}_1}\frac{\mathbf{p}_1}{2m}\right) \end{aligned} \tag{5.7b}$$

$$\begin{aligned} V(t) = \frac{e}{c}\int \frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3}\sum_{\lambda=\{1,2\}} \Bigg(&\underbrace{\alpha\left(k,\lambda\right)\tilde{\mathbf{j}}\left(-\mathbf{k}\right)\cdot\boldsymbol{\epsilon}\left(k,\lambda\right)}_{V} e^{-i\omega_k t} \\ &+ \underbrace{\alpha^*\left(k,\lambda\right)\tilde{\mathbf{j}}(\mathbf{k})\cdot\boldsymbol{\epsilon}^*\left(\mathbf{k},\lambda\right)}_{V^*} e^{i\omega_k t}\Bigg) \end{aligned} \tag{5.7c}$$

5.2 Induced emission and absorption

Consider atom in external (classical) electromagnetic field. Compute transition probability/rate of state ψ_0 into $\psi_n (n \neq 0)$ by absorption of electromagnetic radiation. From section 4.3 for a single mode $(k\lambda)$

$$\Gamma_{10}\left(\mathbf{k},\lambda\right) = \frac{2\pi}{\hbar}\delta\left(E_n - E_0 - \hbar\omega\right)\frac{e^2}{c^2}\left|\alpha\left(k,\lambda\right)\right|^2 \underbrace{\left|\left\langle\psi_n\right|\tilde{\mathbf{j}}\left(-\mathbf{k}\right)\cdot\boldsymbol{\epsilon}\left(\mathbf{k},\lambda\right)\left|\psi_0\right\rangle\right|^2}_{\left|V_{n0}\right|^2} \tag{5.8a}$$

For incoherent radiation (nointerference effects)

$$\begin{aligned}\Gamma_{n0} &= \int\frac{\mathrm{d}^3k}{\left(2\pi\right)^3}\sum_\lambda\Gamma_{n0}\left(\mathbf{k},\lambda\right)\\ &= \int\frac{\mathrm{d}\omega\,' w}{\left(2\pi c\right)^3}\int\mathrm{d}\Omega\sum_\lambda\Gamma_{n0}\left(\mathbf{k},\lambda\right)\\ &= \int\frac{2\pi}{\left(\hbar c\right)^2}\frac{\omega_{n0}^2}{\left(2\pi c\right)^3}\sum_\lambda\left|\alpha\right|^2\left\langle\psi_n\right|\mathbf{j}\cdot\text{''}\left|\psi_0\right\rangle J^2\,\mathrm{d}\Omega\left(\hat{k}\right)\end{aligned} \tag{5.8b}$$

the reverse process: induced emission

$$\begin{aligned}\Gamma_{on} &= \frac{2\pi e^2}{\left(\hbar c\right)^2}\frac{\omega_{n0}^2}{\left(2\pi c\right)^3}\sum\left|\alpha^*\right|^2\left|\left\langle\psi_0\right|j\left(\mathbf{k}\right)\cdot\boldsymbol{\epsilon}(k)\left|\psi_n\right\rangle\right|^2\\ &= \Gamma_{n0}\end{aligned} \tag{5.8c}$$

where

$$\left\langle\psi_0\right|j(\mathbf{k}\cdot\boldsymbol{\epsilon}(k))\left|\psi_n\right\rangle^2 = \left|\left\langle\psi_0\right|\mathbf{j}\left(-\mathbf{k}\right)\boldsymbol{\epsilon}(\mathbf{k})\left|\psi_0\right\rangle\right|^2 \tag{5.8d}$$

Aside: there is a 3rd process: spontaneous emmission (without external field)

5.3 Dipole approximation and selection rules

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

$$\begin{aligned}j\left(\mathbf{k}\right) &= \frac{1}{2m}\left(\mathbf{p}e^{-i\mathbf{k}\cdot\mathbf{r}}] + e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}\right)\\ &= \frac{\mathbf{p}}{m}\end{aligned} \tag{5.9a}$$

with Dipole approximation

$$e^{-i\mathbf{k}\mathbf{r}} = 1 - i\mathbf{k}\mathbf{r} + \dots \tag{5.9b}$$

$$k \sim \frac{1}{\lambda}, \quad \text{for visible light} \sim \left(10 \times 10^{-7}\,\mathrm{m}\right)^{-1} \tag{5.9c}$$

$$\begin{aligned} r &\sim \text{size of atom} \\ &\sim \text{Bohr radius} \\ &\sim 10 \times 10^{-10}\,\mathrm{m} \end{aligned} \tag{5.9d}$$

$$\begin{aligned} \mathbf{j} \cdot \mathbf{A} &\to \text{Dipole approx.} \\ : \mathbf{j} &= \frac{\mathbf{p}}{m} \end{aligned} \tag{5.9e}$$

(radiation filed $\sim$ constant within atom)

Aside: this is equivalent to a term

$$e\mathbf{r} \cdot \mathbf{E} = -\mathbf{d} \cdot \mathbf{E} \tag{5.9f}$$

with $\mathbf{d}$ dipole moment

$$\mathbf{d} \equiv -e\mathbf{r} \tag{5.9g}$$

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

Proof:

$$\begin{aligned} [r_x, H_0] &= \left[r_x, \frac{\mathbf{p}^2}{2m}\right] \\ &= \frac{1}{2m}\left([r_x, \mathbf{p}]\,\mathbf{p} + \mathbf{p}\,[r_x, p]\right) \end{aligned} \tag{5.10a}$$

with

$$[r_x, \mathbf{p}] = \sum_y i\hbar\delta_{xy}p_y \tag{5.10b}$$

$$[r_x, H_0] = \frac{p_x}{m} i\hbar \tag{5.10c}$$

$$[r, H_0] = i\hbar\frac{\mathbf{p}}{m} \tag{5.10d}$$

emission

$$\begin{aligned} \langle\psi_0|\, e\mathbf{r} \cdot \mathbf{E}\, |\psi_n\rangle &= -\frac{e}{c}\langle\psi_0|\, \mathbf{r} \cdot \dot{\mathbf{A}}\, |\psi_n\rangle \\ &= -\frac{e}{c} i\omega \langle\psi_0|\, \mathbf{r} \cdot \mathbf{A}\, |\psi_n\rangle \\ &= -\frac{e}{c}\frac{i}{\hbar}(E_n - E_0)\langle\psi_0|\, \mathbf{r} \cdot \mathbf{A}\, |\psi_n\rangle \\ &= -\frac{e}{c}\frac{i}{\hbar}\langle\psi_0|\, [\mathbf{r}, H_0] \cdot \mathbf{A}\, |\psi_n\rangle \end{aligned} \tag{5.10e}$$

using Eq. 5.10d

$$\begin{aligned} \langle\psi_0| e\mathbf{r}\cdot\mathbf{E}\,|\psi_n\rangle &= -\frac{e}{c}\,\langle\psi_0|\,\frac{\mathbf{p}}{m}\cdot\mathbf{A}\,|\psi_n\rangle \\ &= \frac{e}{c}\,\langle\psi_0|\,\mathbf{j}\cdot\mathbf{A}\,|\psi_n\rangle \end{aligned} \tag{5.10f}$$

Proof (alternative): Make gauge trafo with

$$\chi(\mathbf{r},t) = -\mathbf{A}(t)\cdot\mathbf{r} \tag{5.11a}$$

$$\mathbf{A}\to\mathbf{A}+\boldsymbol{\nabla}\xi = 0 \tag{5.11b}$$

$$0=\Phi\to\Phi-\frac{1}{c}\dot{\chi} = -\frac{1}{c}\dot{\mathbf{A}}\cdot\mathbf{r} = -\mathbf{E}\cdot\mathbf{r} \tag{5.11c}$$

$$H - e\Phi = -e\mathbf{r}\mathbf{E} \tag{5.11d}$$

Atomic transitions are only possible if

$$\left\langle\psi_{n'\ell'm_\ell'}\middle|\,\mathbf{r}\,\middle|\psi_{n\ell m_\ell}\right\rangle \neq 0 \tag{5.12a}$$

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

$$\int \mathrm{d}\Omega\,\left(Y_{\ell'}^{m_{\ell'}}(\theta,\phi)\right)^* \begin{pmatrix} x+iy \\ x-iy \\ z \end{pmatrix} \mathcal{Y}_\ell^{m_\ell}(\theta,\phi) \tag{5.13a}$$

this is most of the time 0 exept if

$$\left\langle\psi_{n'\ell'm_\ell'}\middle|\,z\,\middle|\psi_{n\ell m_\ell}\right\rangle \neq 0,\quad \ell'=\ell\pm1, m_\ell'=m_\ell \tag{5.13b}$$

$$\left\langle\psi_{n'\ell'm_\ell'}\middle|\,x\pm iy\,\middle|\psi_{n\ell m_\ell}\right\rangle \neq 0,\quad \ell'=\ell\pm1, m_\ell'=m_\ell\pm1 \tag{5.13c}$$

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

$$\Delta\ell = \pm1 \tag{5.13d}$$

$$\Delta m = 0, \pm1 \tag{5.13e}$$

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 $j=0\to j=0$ (total angular momentum conservation)

Chapter 6

Potential scattering

We consider

$$H = H_0 + V(r) \tag{6.1a}$$

with

$$\lim_{r \to \infty} rV(r) = 0, \quad \text{(i.e. \textit{not} Coloumb)} \tag{6.1b}$$

V is restricted to “small” region.
Want to find stationary solutions

$$\psi(\mathbf{r}, t) = e^{-\frac{i}{\hbar}Et}\psi(\mathbf{r}), \quad \text{for } r \to \infty \tag{6.1c}$$

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

6.1 Elastic scattering and cross sections

we are looking for solutions to

$$(H_0 + V)|\psi\rangle = E|\psi\rangle \tag{6.2a}$$

$$\begin{aligned} E_{\text{in}} &= E_{\text{out}} \\ &= \frac{p^2}{2m} \\ &= \frac{\hbar^2 k^2}{2m} \end{aligned} \tag{6.2b}$$

of the form

$$r \to \infty \tag{6.2c}$$

$$\begin{aligned} \psi_k(\mathbf{r}) &\to \psi_{\text{in}}(\mathbf{r}) + \psi_{\text{sc}}(\mathbf{r}) \\ &= e^{i\mathbf{k}\mathbf{r}} + f(\theta, \phi)\frac{e^{ikr}}{r} \end{aligned} \tag{6.2d}$$

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

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{N}{F} \tag{6.3}$$

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 $|\psi_{\mathrm{in}}|^2 = 1$ (1 part/volume),

$$\begin{aligned} F &= V \\ &= \frac{p}{m} \\ &= \frac{\hbar k}{m} \end{aligned} \tag{6.4a}$$

outgoing:

$$\begin{aligned} \mathbf{j} &= \dots \\ &= \frac{\hbar k}{m} \left| f(\theta, \phi) \right|^2 \frac{\mathbf{e}_r}{r^2} \end{aligned} \tag{6.4b}$$

$$\Rightarrow \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left| f(\theta,' i) \right|^2 \tag{6.4c}$$

total cross section

$$\sigma = \int \mathrm{d}\Omega \, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \tag{6.4d}$$

6.2 Partial-wave analysis

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

$$\psi_k(r, \theta) = \sum_{\ell=0}^{\infty} R_\ell(kr) \, P_\ell(\cos\theta) \tag{6.5a}$$

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

$$f(\theta) = \sum_{\ell=0}^{\infty} P_\ell(k) \, P_\ell(\cos\theta) \tag{6.5b}$$

→ equation for R_ℓ:

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\ell\,(\ell+1)}{r^2} + 2m\,(V(r)-E)\,R_\ell\,(kr) = 0 \tag{6.5c}$$

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

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

$$j_\ell\,(\rho) \equiv (-\rho)^\ell \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell \frac{\sin\rho}{\rho} \tag{6.6a}$$

Spherical Neumann function:

$$n_\ell\,(\rho) = -\,(-\rho)^\ell \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell \frac{\cos\rho}{\rho} \tag{6.6b}$$

$$j_\ell\,(\rho) \xrightarrow{\rho\,\to 0} \rho^\ell \xrightarrow{\rho\,\to\infty} \frac{1}{\rho}\sin\left(\rho - \frac{\pi\ell}{2}\right) \tag{6.7a}$$

$$n_\ell(\rho) \xrightarrow{\rho\,\to 0} \frac{1}{\rho^{\ell-1}} \xrightarrow{\rho\,\to\infty} -\frac{1}{\rho}\cos\left(\rho - \frac{\pi\ell}{2}\right) \tag{6.7b}$$

$$h_\ell = j_\ell \pm i n_\ell \tag{6.7c}$$

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

$$\begin{aligned} R_\ell(r) &\sim j_\ell(\rho) \\ &= j_\ell\,(kr) \end{aligned} \tag{6.8a}$$

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

$$\begin{aligned} R_\ell(r) &= B_\ell(k) j_\ell(kr) + C_\ell n_\ell(kr) \xrightarrow{r\to\infty} B_\ell(k)\frac{1}{kr}\sin\left(kr - \frac{\pi\ell}{2}\right) \\ &\quad - C_\ell(k)\frac{1}{kr}\cos\left(kr - \frac{\pi\ell}{2}\right) \\ &= \frac{1}{kr}A_\ell(k)\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right), \\ &\quad A_\ell = \sqrt{B_\ell^2 + C_\ell^2},\ \text{phase shift } \tan\delta_\ell = -\tfrac{C_\ell(k)}{B_{\ell(k)}} \end{aligned} \tag{6.8b}$$

note: for $V = 0$:

$$R_\ell \sim j_\ell\,(kr) \tag{6.9a}$$

i.e. C_ℓ and $\delta_\ell = 0$

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

$$\psi_k \to e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta) e^{ikr} \frac{1}{r} \tag{6.10}$$

central potential

$$\psi_k = \sum_{\ell=0}^{\infty} R_\ell (kr) P_\ell (\cos\theta) \tag{6.11a}$$

$$f_k = \sum_{\ell=0}^{\infty} f_\ell(k) P_\ell (\cos\theta) \tag{6.11b}$$

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

$$\begin{aligned} R_\ell(kr) &\overset{r\to\infty}{\simeq} \frac{1}{kr}\left(B_\ell \sin\left(kr - \frac{\ell\pi}{2}\right) + C_\ell \cos\left(kr - \frac{\ell\pi}{2}\right)\right) \\ &= \frac{1}{kr} A_\ell \sin\left(kr - \frac{\ell\pi}{2} + \underbrace{\delta_\ell(k)}_{\text{phase shift}} \right) \end{aligned} \tag{6.11c}$$

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

$$\psi_{j\ell m_\ell}(r,\phi,\theta) = C_{J\ell}(kr) Y_\ell^{m_\ell}(\theta,\phi)\,, \quad E = \tfrac{\hbar^2 k^2}{2m} \tag{6.12a}$$

Form a basis, expand

$$e^{i\mathbf{kr}} = e^{ikr\cos\theta} \tag{6.12b}$$

in this basis

$$e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty} \sum_{m_\ell}^{\ell} C_{\ell m_\ell} j_\ell (kr) Y_\ell^{m_\ell}(\theta,\phi) \tag{6.12c}$$

having no ϕ dependence

$$\rightsquigarrow e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty} a_\ell j_\ell(kr) P_\ell (\cos\theta) \tag{6.12d}$$

fix coefficient a_ℓ (use orthogonality)

$$e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell j_\ell(kr)\, P_\ell(\cos\theta) \tag{6.12e}$$

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

$$\frac{1}{kr} A_\ell \sin\left(kr - \frac{\pi\ell}{2} + \delta_\ell\right) = (2\ell+1)\, i^\ell \frac{1}{kr} \sin\left(kr - \frac{\pi\ell}{2}\right) + f_\ell \frac{e^{ikr}}{r} \tag{6.12f}$$

$$\begin{aligned} \frac{A_\ell}{2i} e^{ikr} e^{-\frac{i\pi\ell}{2}} e^{i\delta_\ell} - \frac{A_\ell}{2i} e^{-ikr} e^{\frac{i\pi\ell}{2}} e^{-i\delta_\ell} &= (2\ell+1)\, i^\ell \frac{1}{2i} e^{ikr} e^{-\frac{i\ell\pi}{2}} \\ &\quad - (2\ell+1)\, i^\ell \frac{1}{2i} e^{-ikr} e^{\frac{i\ell\pi}{2}} + k f_\ell e^{ikr} \end{aligned} \tag{6.12g}$$

$$A_\ell = (2\ell+1)\, i^\ell e^{i\delta_\ell} \tag{6.12h}$$

$$\begin{aligned} f_\ell &= \frac{2\ell+1}{2ik}\left(e^{2i\delta_\ell} - 1\right) \\ &= \frac{2\ell+1}{k} e^{i\delta_\ell} \sin(\delta_\ell) \end{aligned} \tag{6.12i}$$

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

$$\begin{aligned} f(\theta) &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} e^{i\delta_\ell} \sin(\delta_\ell)\, P_\ell(\cos\theta) \\ &= \sum_{\ell=0}^{\infty} f_\ell P_\ell(\cos\theta) \end{aligned} \tag{6.12j}$$

Total cross section

$$\begin{aligned} \sigma_{\mathrm{tot}} &= \int \mathrm{d}\Omega \, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \\ &= \int \mathrm{d}\Omega \, |f(\theta)|^2 \\ &= 2\pi \int_{-1}^{1} \mathrm{d}\cos\theta \sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} f_\ell f_{\ell'}^* P_\ell(\cos\theta)\, P_\ell(\cos\theta) \end{aligned} \tag{6.13a}$$

use

$$\int \mathrm{d}\cos\theta \, P_\ell(\cos\theta)\, P_{\ell'}(\cos\theta) = \frac{2}{2\ell+1} \delta_{\ell\ell'} \tag{6.13b}$$

$$\begin{aligned}\Rightarrow \sigma_{\text{tot}} &= \sum_{\ell=0}^{\infty} 4\pi \frac{2\ell+1}{k^2} \sin^2\left(\delta_{/ell}\right) \\ &\equiv \sum_{\ell=0}^{\infty} \sigma_\ell\end{aligned} \tag{6.13c}$$

6.2.1 The optical theorem

$$\begin{aligned}\operatorname{im}\left(f\left(\theta=0\right)\right) &= \Im\left(\sum_{\ell=0}^{\infty} f_\ell\right) \\ &= \operatorname{im}\left(\sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} e^{i\delta_\ell} \sin\left(\delta_\ell\right)\right) \\ &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} \sin^2\left(\delta_\ell\right)\end{aligned} \tag{6.14a}$$

$$\begin{aligned}\Rightarrow \sigma_{\text{tot}} &= \frac{4\pi}{k} \operatorname{im}\left(f\left(\theta\right.\right. \\ &\left.\left.= 0\right)\right)\end{aligned} \tag{6.14b}$$

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 $b > a$

$$\begin{aligned}L &\simeq \ell \cdot \hbar \\ &= b \cdot P \\ &= b \cdot \hbar \cdot k\end{aligned} \tag{6.15}$$

no scattering for

$$\begin{aligned}b &= \frac{\ell}{k} \\ &> a\end{aligned} \tag{6.16}$$

6.3 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)

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \frac{Z_1 Z_2 e^2}{r}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{6.17}$$

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

$$\lim_{r\to\infty} |\psi(\mathbf{r})|^2 = 0 \tag{6.18}$$

- scattering $E > 0$ with different

$$\nabla^2 = \frac{4}{\xi+\eta}\left(\partial_\xi \xi \partial_\xi + \partial_\eta \eta \partial_\eta\right) + \underbrace{\frac{1}{\xi\eta}\frac{\partial^2}{\partial\varphi^2}}_{\spadesuit} \tag{6.19}$$

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

$$\gamma = \frac{m Z_1 Z_2 e^2}{\hbar^2 k} \tag{6.20a}$$

$$\begin{aligned}\psi_\ell(r) \xrightarrow[r\to\infty]{\mathbf{k}=k\mathbf{e}_z} & \underbrace{e^{i(kz+\gamma\log 2k(r-z))}}_{\text{distorted plane wave}} \\ & -\frac{\gamma}{2k\sin^2\frac{\vartheta}{2}}\frac{\Gamma(1+\gamma)}{\Gamma(1-i\gamma)} e^{-i\gamma\log\left(\sin\frac{2\vartheta}{2}\right)} \underbrace{\frac{e^{i(kr-\gamma\log 2kr)}}{2}}_{\text{distorted outgoing plane wave}}\end{aligned} \tag{6.20b}$$

This looks the same as

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} + f(\vartheta)\frac{e^{ikr}}{r} \tag{6.21}$$

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

$$\begin{aligned} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= |f_c(\vartheta)| \\ &= \frac{\gamma}{4k^2 \sin^4 \frac{\vartheta}{2}} \\ &= \left(\frac{Z_1 Z_2 e^2}{4E}\right)^2 \frac{1}{\sin^4 \frac{\vartheta}{2}} \end{aligned} \tag{6.22}$$

$\to$ $\to$ 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)

$$\left[-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{6.23}$$

-

$$\begin{aligned} \mu &= \frac{m_1 m_2}{m_1 + m_2} \\ &= \frac{m}{2}, \quad \text{reduced mass} \end{aligned} \tag{6.24}$$

$$V \sim \text{interaction potential} \tag{6.25}$$

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_A - \mathbf{r}_B \\ &\sim \text{relative coordinate} \end{aligned} \tag{6.26}$$

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

$$\psi_{\text{sym/antysym}} = \left(e^{i\mathbf{kr}} \pm e^{-i\mathbf{kr}}\right) + \left(f(\vartheta) \pm f(\pi - \vartheta)\right)\frac{e^{ikr}}{r} \tag{6.27}$$

Example: Coulomb scattering of two protons (spin $\frac{1}{2}$, fermions $\rightarrow$ 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.

$$\rightarrow \sigma_{\text{sing}} = \left|f_\ell(\vartheta) + f_c\left(\pi - \vartheta\right)\right|^2 \tag{6.28}$$

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

$$\rightarrow \sigma_{\text{trp}} = \left|f_c\left(\vartheta\right) - f_c\left(\pi - \vartheta\right)\right|^2 \tag{6.29}$$

Unpolarized cross-section:

$$\begin{aligned}\sigma &= \frac{1}{4}\left|f_c(\vartheta) + f\left(\pi - \vartheta\right)\right|^2 + \frac{3}{4}\left|f_c(\vartheta) - f_c(\pi - \vartheta)\right|^2 \\ &= \left|f_c\left(\vartheta\right)\right|^2 + \left|f_c\left(\pi - \vartheta\right)\right|^2 \\ &\quad - \frac{1}{2}\left(f_c(\vartheta)f_c^*\left(\pi - \vartheta\right) + f_c^*(\vartheta)f_c\left(\pi - \vartheta\right)\right) \overset{Z_1 = Z_2 = 1}{=} \left(\frac{e}{4E}\right)^2 \left(\underbrace{\frac{1}{\sin\frac{4\theta}{2}} + \frac{1}{\cos^4\frac{\vartheta}{2}}}_{\text{classical}} \right. \\ &\qquad \left. - \frac{\cos\left(\gamma \log\left(\tan^2\frac{\vartheta}{2}\right)\right)}{\sin^2\frac{\vartheta}{2}\cos^2\frac{\vartheta}{2}}\right)\end{aligned} \tag{6.30}$$

Mott scattering formula

6.4 Lippman- Schwinger equation & Green's function

Again:

$$E_k = \frac{\hbar^2 k^2}{2m} \tag{6.31a}$$

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_k\right)\psi_k(\mathbf{r}) = V(\mathbf{r})\psi(\mathbf{r}) \tag{6.31b}$$

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

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_k\right) g_k(\mathbf{r}) = \delta(\mathbf{r}) \tag{6.32}$$

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

$$\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} + \int \mathrm{d}^3\,\mathbf{r}' g_k(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{6.33}$$

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

$$g_k(\mathbf{r}) = \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} e^{-i\mathbf{qr}} \tilde{g}_k(\mathbf{q}) \tag{6.34}$$

We get

$$\begin{aligned}\left(\frac{\hbar^2}{2m}\nabla^2 + E_k\right) g_k(\mathbf{r}) &= \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3}\left(-\frac{\hbar^2}{2m}q^2 + \frac{\hbar^2}{2m}k^2\right) e^{-i\mathbf{qr}}\tilde{g}_k(\mathbf{q}) \\ &= \delta(\mathbf{r}) \\ &= \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} e^{-i\mathbf{qr}}\end{aligned} \tag{6.35a}$$

$$\begin{aligned}\Rightarrow \tilde{g}_k(\mathbf{q}) &= \frac{2m}{\hbar^2}\frac{1}{k^2-q^2} \\ &= \left(E_k - \frac{\hbar^2 q^2}{2m}\right)^{-1}\end{aligned} \tag{6.35b}$$

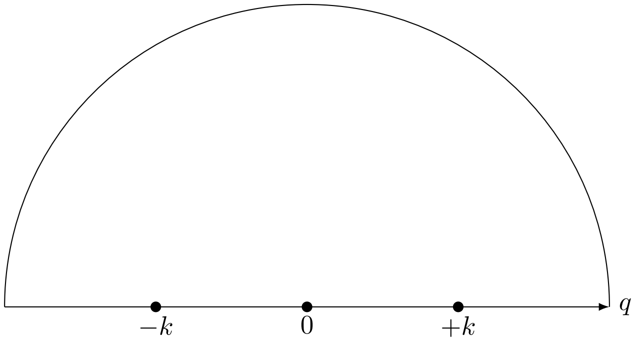

Figure 6.1:

$$
\begin{aligned}
g_k(r) &= \frac{1}{(2\pi)^3}\int_0^\infty \mathrm{d}q \int_0^{2\pi} |\mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}\cos\vartheta \\
&\qquad \cdot q^2 \frac{2m}{\hbar^2}\frac{1}{k^2-q^2} e^{-iqr\cos\vartheta} \qquad (6.35c)\\
&= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2} \\
&= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty \mathrm{d}q \frac{q^2}{iqr}\frac{1}{k^2-q^2}\left(e^{iqr} - \underbrace{e^{-iqr}}_{\spadesuit}\right) \\
&= \frac{m}{2\pi^2\hbar^2}\frac{1}{ir}\int_{-\infty}^{\infty} \mathrm{d}q \frac{q}{k^2-q^2} e^{iqr}
\end{aligned}
$$

$\spadesuit$:

$$
\int_0^\infty \mathrm{d}q \xrightarrow{q \to -1} -\int_0^{-\infty} = \int_{-\infty}^{0} \mathrm{d}q \tag{6.36}
$$

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

$$
\begin{aligned}
q &= q_{R\ell} + iq_{\ell m} \\
&\rightarrow e^{iqr} \\
&= e^{iq_{R\ell}r}e^{-q_{\ell m}r}
\end{aligned}
\tag{6.37}
$$

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:

$$
\begin{aligned}
g_k^+(r) &= 2\pi i \frac{m}{2\pi^2\hbar^2}\frac{1}{ir} Res_{q=k}\frac{-q}{(q-k)(q+k)}e^{iqr} \\
&= -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}
\end{aligned}
\tag{6.38a}
$$

For negative point inside and positive point outside curve:

$$
g_k^-(r) = -\frac{m}{2\pi\hbar^2}\frac{e^{-ikr}}{r}
\tag{6.38b}
$$

for both points inside:

$$
g_k^+(r) + g_k^-(r)
\tag{6.38c}
$$

Both points outside

$$
0
\tag{6.38d}
$$

$g_k^+ \sim$ outgoing spherical wave

$g_k^- \sim$ incoming spherical wave

What we need is g_k^+!

$$
\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} - \int \mathrm{d}^3\mathbf{r}' \frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')\psi(\mathbf{r}')
\tag{6.39}
$$

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

$$
\begin{aligned}
|\mathbf{r}-\mathbf{r}'| &\xrightarrow{|\mathbf{r}|\to\infty} r\left(1 - \frac{r'}{r}\cos\vartheta + \mathcal{O}\left(\left(\frac{r'}{r}\right)\right)\right) \\
&= r - \frac{\mathbf{r}\mathbf{r}'}{r'} \\
&= r - \hat{e}_r\cdot\mathbf{r}'
\end{aligned}
\tag{6.40a}
$$

We get:

$$
\begin{aligned}
\psi_k(\mathbf{r}) &= e^{i\mathbf{kr}} - \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}' \frac{e^{ikre^{-ik\mathbf{e}_r\mathbf{r}'}}}{r} \times V(\mathbf{r}')\psi_k(\mathbf{r}') \\
&= e^{ikr} + f(\mathbf{r})\frac{e^{ikr}}{r}
\end{aligned}
\tag{6.40b}
$$

where

$$
f(\mathbf{r}) = \frac{-m}{2\pi\hbar}\int \mathrm{d}^3\mathbf{r}' \underbrace{e^{-ik\hat{\mathbf{e}}_r\cdot\mathbf{r}'}}_{\spadesuit} V(\mathbf{r}')\psi_k(\mathbf{r}')
\tag{6.40c}
$$

♠: $\vartheta = \angle(\mathbf{k}, \mathbf{r})$ dependence. If $V(\mathbf{r}') = V(r) \rightsquigarrow f(\vartheta, \varphi)$.

This is still a formal solution because ψ_k is on the right hand side. $\rightsquigarrow$ Proceed as in perturbation theory and get another expansion.

6.5 The Born approximation

Formal solution

$$\psi_k(\mathbf{r}) = e^{i\mathbf{kr}} + \int \mathrm{d}^3\mathbf{r}'\, g_k^+(\mathbf{r} - \mathbf{r}')\, V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{6.41a}$$

$$g_k^+(\mathbf{r} - \mathbf{r}') = -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \tag{6.41b}$$

$$f = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}' e^{-ik\mathbf{e}_r\cdot\mathbf{r}'} V(\mathbf{r}')\psi_k(\mathbf{r}') \tag{6.41c}$$

Solve this "pertubatively" by iteration.

$$\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{n=1}^{\infty}\int \mathrm{d}^3\mathbf{r}'\, K_(\mathbf{r}, \mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'} \tag{6.42a}$$

$$K_1(\mathbf{r}, \mathbf{r}') = g_k^+(\mathbf{r} - \mathbf{r}')\, V(\mathbf{r}'), \quad \sim V^1 \tag{6.42b}$$

$$\begin{aligned} K_n(\mathbf{r}, \mathbf{r}') &= \int \mathrm{d}^3\mathbf{r}''\, K_1(\mathbf{r}, \mathbf{r}'')\, K_{n-1}(\mathbf{r}'', \mathbf{r}'), \quad \sim V^n \\ &= \int \left(\prod_{i=1}^{n} \mathrm{d}^3\mathbf{r}_i\right) g_k^+(\mathbf{r} - \mathbf{r})\, V(\mathbf{r}_n) g^+(\mathbf{r}_n - \mathbf{r}_{n-1}) \ldots g_k^+(\mathbf{r}_2 \\ &\qquad - \mathbf{r}_1)\, V(\mathbf{r}_1) \end{aligned} \tag{6.42c}$$

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

$$\psi_k^{(1)}(\mathbf{r}) = e^{ikz} \underbrace{-\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}' V(\mathbf{r}') e^{ik(\mathbf{e}_z - \mathbf{e}_r)\cdot\mathbf{r}'}}_{f^{(1)}(\theta,\phi)} \frac{e^{ikr}}{r} \tag{6.43}$$

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

$$\begin{aligned} \mathbf{q} &\equiv k(\mathbf{e}_z - \mathbf{e}_r) \\ &= \mathbf{k} - \mathbf{k}', \quad \text{momentum transfer} \end{aligned} \tag{6.44a}$$

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

$$\begin{aligned} f^{(1)}(\theta,\phi) &= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}\phi \int_{-1}^{1} \mathrm{d}\cos\vartheta \int \mathrm{d}r'\, V(r') e^{iqr'\cos\vartheta} \\ &= -\frac{m}{\hbar^2}\int r'^2\,\mathrm{d}r' \frac{2\sin(qr')}{qr'} V(r') \end{aligned} \tag{6.45a}$$

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2 q}\int \mathrm{d}r'\, r' V(r') \sin(qr')\,, \quad q = 2k\sin\tfrac{\theta}{2} \tag{6.45b}$$

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

Example: Yukawa potential:

$$V(r) = V_0 \frac{e^{-\mu r}}{r}, \quad \mu \sim \text{range of interaction} \tag{6.46a}$$

$$\begin{aligned} f^{(1)} &= -\frac{2m}{\hbar^2 q} V_0 \underbrace{\int_0^\infty \mathrm{d}r' e^{-\mu r'} \sin(qr')}_{q/(\mu^2+q^2)} \\ &= -\frac{2m}{\hbar^2}\frac{V_0}{\mu^2+q^2} \end{aligned} \tag{6.46b}$$

$$\begin{aligned} \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(1)} &= \left| f^{(1)}(\theta)\right|^2 \\ &= \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{\left(\mu^2 + 2k^2(1-\cos\theta)\right)^2} \end{aligned} \tag{6.46c}$$

total cross section

$$\begin{aligned} \sigma_{\text{tot}}^{(1)} &= 2\pi \int_{-1}^{1} \mathrm{d}\cos\theta \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{\left(\mu^2 + 2k^2(1-\cos\theta)\right)^2} \\ &= 2\pi \left(\frac{2mV_0}{\hbar^2}\right) \frac{2}{\mu^4 + 4k^2\mu^2} \end{aligned} \tag{6.46d}$$

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

$$V(\mathbf{r}) = \frac{V_0}{r}, \quad \text{(Coulomb)} \tag{6.47a}$$

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(1)}_{\text{Coulomb}} = \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{\left(2k^2(1-\cos\theta)\right)} \tag{6.47b}$$

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

Chapter 7

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)

7.1 Dynamics of scattering

Start from time dependent Schrödinger

$$i\hbar\partial_t |\psi, t\rangle = H |\psi, t\rangle \tag{7.1a}$$

$$H = H_0 + V \tag{7.1b}$$

$$\ldots = \ldots \tag{7.1c}$$

$$\begin{aligned}(i\hbar\partial_t - H_0) |\psi, t\rangle &= V |\psi, t\rangle \\ &= |\chi, t\rangle\end{aligned} \tag{7.1d}$$

Definition 7.1.1: Green operation $G_0(t, t')$ through

$$(i\hbar\partial_t - H_0) G_0(t, t') = \delta(t - t') \cdot \mathbf{1}, \quad (\leftarrow \text{operators}) \tag{7.2}$$

inhomogeneous differential equation in t

$$G_0^+(t, t') = -\frac{i}{\hbar}\theta(t - t') e^{-\frac{i}{\hbar}H_0(t-t')} \tag{7.3a}$$

$$G_0^-(t, t') = +\frac{i}{\hbar} \tag{7.3b}$$

Proof:

$$\begin{aligned}
i\hbar\partial_t G_0^+(t-t') &= i\hbar\left(-\frac{i}{\hbar}\right)\partial_t\theta(t-t')\,e^{-\frac{i}{\hbar}H_0\left(t-t'\right)} \\
&= \delta(t-t')\,e^{-\frac{i}{\hbar}H_0\left(t-t'\right)} \\
&\quad+\theta(t-t')\left(-\frac{i}{\hbar}H_0\right)e^{-\frac{i}{\hbar}H_0\left(t-t'\right)} \\
&= \delta(t-t') + H_0 G_0^+(t-t')
\end{aligned} \tag{7.4a}$$

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

$$G_0^{\pm}(t,t') = G_0^{pm}(t-t') \tag{7.5a}$$

Write solution to Schrödinger

$$\left|\psi^{\pm},t\right\rangle = \left|\psi^0,t\right\rangle + \int \mathrm{d}t' G_0^{\pm}(t-t')\,V\left|\psi^{\pm},t'\right\rangle \tag{7.5b}$$

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

$$(i\hbar\partial_t - H_0)\left|\psi_0,t\right\rangle = 0 \tag{7.5c}$$

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

$$\begin{aligned}
G_0^+(E) &= \int_{-\infty}^{\infty}\mathrm{d}t\,e^{\frac{i}{\hbar}Et}G_0^+(t) \\
&= -\frac{i}{\hbar}\int_0^{\infty}\mathrm{d}t\,e^{\frac{i}{\hbar}Et}e^{-\frac{i}{\hbar}H_0 t}
\end{aligned} \tag{7.6a}$$

with

$$G_0^+(t) = G_0^+(t,t'=0) \tag{7.6b}$$

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

$$\begin{aligned}
G_0^{\pm} &= \frac{1}{E-H_0\pm i0^+} \\
&\equiv \left(E-H_0\pm i0^+\right)^{-1}
\end{aligned} \tag{7.6c}$$

$|\psi^{\pm}, t\rangle$ 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)

$$\to \left|\psi^0_\alpha, t\right\rangle \leftrightarrow \left|\psi^{\pm}_\alpha, t\right\rangle \tag{7.7a}$$

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

$$\begin{aligned}\underbrace{\int \mathrm{d}t\, e^{\frac{i}{\hbar}Et}\left|\psi^{\pm}_\alpha, t\right\rangle}_{\left|\psi^{\pm}_\alpha(E)\right\rangle \to \left|\psi^{\pm}_\alpha\right\rangle} &= \underbrace{\int \mathrm{d}t\, e^{\frac{i}{\hbar}Et}\left|\psi^0_\alpha, t\right\rangle}_{\left|\psi^0_\alpha(E)\right\rangle \sim \left|\psi^0_\alpha\right\rangle} \\ &\quad + \int \mathrm{d}t\, e^{\frac{i}{\hbar}Et}\underbrace{\int \mathrm{d}t'\, G^{\pm}_0\left(t-t'\right)}_{t\to t+t'} V\left|\psi^{\pm}_\alpha, t\right\rangle\end{aligned} \tag{7.7b}$$

$$\int \mathrm{d}t\, e^{\frac{i}{\hbar}Et} G^+_0(t) = G^+_0(E) \tag{7.7c}$$

$$V\left|\psi^{\pm}_\alpha(E)\right\rangle = \int \mathrm{d}t'\, e^{\frac{i}{\hbar}Et'} V\left(\psi^{\pm}_\alpha(E)\right) \tag{7.7d}$$

$$\left|{}^{\pm}_{\alpha}\right\rangle = \left|\psi^0_\alpha\right\rangle + G^{\pm}_0 V\left|\psi^{\pm}_\alpha\right\rangle, \quad \text{(Lippmann-Schwinger)} \tag{7.8a}$$

Solution:

$$\begin{aligned}\left|\psi^{\pm}_\alpha\right\rangle &= \left(1 - G^{\pm}_0 V\right)^{-1}\left|\psi^0_\alpha\right\rangle \\ &= \frac{1}{\left(G^{\pm}_0\right)^{-1} - V}\left(G^{pm}_0\right)^{-1}\left|\psi^0_\alpha\right\rangle \\ &= \frac{1}{E_\alpha - H_0 \pm i0^+ - V}\left(E_{\cdot ?a} - H_0 \pm i0^+ - V + V\right)\left|\psi^0_\alpha\right\rangle \\ &= \underbrace{\frac{1}{E_\alpha - H \pm i0^+}}_{G^{\pm}E_\alpha}\left(E_\alpha - H + V \pm i0^+\right)\left|\psi^0_\alpha\right\rangle \\ &= \left(1 + G^{\pm}V\right)\left|\psi^0_\alpha\right\rangle\end{aligned} \tag{7.9a}$$

$$\psi^{\pm}_\alpha = \left(1 + G^{\pm}V\right)\left|\psi^0_\alpha\right\rangle \tag{7.9b}$$

can also be obtained from (exercise 2)

$$\left|\psi^{\pm}, t\right\rangle = \lim_{t' \to \mp\infty} i\hbar G^+\left(t - t'\right)\left|\psi_0, t'\right\rangle \tag{7.9c}$$

7.2 Møller operators & scattering operator

α: Complete set of quantum numbers

$$H_0 \left|\psi_\alpha^0\right\rangle = E_\alpha \left|\psi_\alpha^0\right\rangle \tag{7.10a}$$

$$H \left|\psi_\alpha^\pm\right\rangle = E_\alpha \left|\psi_\alpha^\pm\right\rangle \tag{7.10b}$$

Consider again

$$\begin{aligned} \left|\psi_\alpha^\pm\right\rangle &= \left|\psi_\alpha^0\right\rangle + \left(E_\alpha - H_0 + \pm O^+\right)^{-1} V \left|\psi_\alpha^\pm\right\rangle \\ &= \left|\psi_\alpha^0\right\rangle + \int \mathrm{d}\beta \, \frac{T_{\beta\alpha} \left|\psi_\beta^0\right\rangle}{E_\alpha - E_\beta \pm i0^+} \end{aligned} \tag{7.10c}$$

$$1 = \int \mathrm{d}\beta \left|\psi_\beta^0\right\rangle\!\left\langle\psi_\beta^0\right| \tag{7.10d}$$

$$T_{\beta\alpha} \equiv \left\langle\psi_\beta^0\right| V \left|\psi_\alpha^\pm\right\rangle \tag{7.10e}$$

Transfer matrix

This state satisfies:

$$\int \mathrm{d}\alpha \, e^{-\frac{i}{\hbar}E_\alpha \tau} f(\alpha) \left|\psi_\alpha^\pm\right\rangle \xrightarrow{\tau \to \mp\infty} \int \mathrm{d}\alpha \, e^{-\frac{i}{\hbar}E_\alpha \tau} f(\alpha) \left|\psi_\alpha^0\right\rangle \tag{7.11a}$$

or

$$e^{-\frac{i}{\hbar}H\tau} \int \mathrm{d}\alpha \, f(\alpha) \left|\psi_\alpha^\pm\right\rangle \xrightarrow{e^{-\frac{i}{\hbar}H_0\tau}} \int \mathrm{d}\alpha \, f(\alpha) \left|\psi_\alpha^0\right\rangle \tag{7.11b}$$

$$\begin{aligned} \Rightarrow \left|\psi_\alpha^\pm\right\rangle &= \lim_{\tau \mp \infty} e^{+\frac{i}{\hbar}H\tau} e^{-\frac{i}{\hbar}H_0\tau} \left|\psi_\alpha^0\right\rangle \\ &= \Omega^\pm \left|\psi_\alpha^0\right\rangle \end{aligned} \tag{7.11c}$$

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:

$$\left\langle \psi_\beta^- \middle| \psi_\alpha^+ \right\rangle = \left\langle \psi_\beta^0 \right| \left(\Omega^-\right)^\dagger \Omega^+ \left| \psi_\alpha^0 \right\rangle \equiv \left\langle \psi_\beta^0 \right| S \left| \psi_\alpha^0 \right\rangle \tag{7.12}$$

$$\begin{aligned} S &= \lim_{\substack{\tau\to\infty\\ \tau\to-\infty}} e^{\frac{i}{\hbar}H_0\tau} e^{\frac{i}{\hbar}H(\tau_0-\tau)} e^{-\frac{i}{\hbar}H_0\tau_0} \\ &= \lim_{\substack{\tau\to\infty\\ \tau_0\to-\infty}} U\left(\tau,\tau_0\right) \\ &= U\left(\infty,-\infty\right) \end{aligned} \tag{7.13}$$

ex 1: sheet 6:

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}\tau}U\left(\tau,\tau_0\right) &= e^{\frac{i}{\hbar}H_0\tau}\left(H-H_0\right)e^{\frac{i}{\hbar}H(\tau_0-\tau)}e^{-\frac{i}{\hbar}H_0\tau_0} \\ &= \underbrace{e^{\frac{i}{\hbar}H_0\tau}Ve^{-\frac{i}{\hbar}H_0\tau}}_{V(\tau)}U\left(\tau,\tau_0\right) \\ &= V(\tau)U\left(\tau,\tau_0\right) \end{aligned} \tag{7.14a}$$

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

$$U\left(\tau,\tau_0\right) = T\left(e^{-\frac{i}{\hbar}\int_{\tau_0}^{\tau}V(\tau)\,\mathrm{d}\tau}\right) \tag{7.15a}$$

and

$$\begin{aligned} S &= U\left(\infty,-\infty\right) \\ &= \mathbf{1} - \frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t_1 V(t_1) + \left(-\frac{i}{\hbar}\right)^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2 V(t_1)V(t_2) + \dots \end{aligned} \tag{7.15b}$$

Note:

$$SS^\dagger = \mathbf{1}, \quad S \text{ operator is unitary} \tag{7.16}$$

S-matrix

$$\begin{aligned} S_{\beta\alpha} &\equiv \left\langle \psi_\beta^0 \right| S \left| \psi_\alpha^0 \right\rangle \\ &= \left\langle \psi_\beta^- \middle| \psi_\alpha^\dagger \right\rangle \end{aligned} \tag{7.17}$$

option 1 insert S operator

1st term:

$$\left\langle\psi_\beta^0\right| \mathbf{1} \left|\psi_\alpha^0\right\rangle = \delta\left(\beta-\alpha\right) \tag{7.18}$$

2nd term

$$\begin{aligned}
&-\frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t_1\left\langle\psi_\beta^0\right| e^{\frac{i}{\hbar}H_0 t} V e^{-\frac{i}{\hbar}H_0 t}\left|\psi_\alpha^0\right\rangle\\
&= -\frac{i}{\hbar}\int \mathrm{d}t e^{-\frac{i}{\hbar}(E_\alpha-E_\beta)t}\left\langle\psi_\beta^0\right| V\left|\psi_\alpha^0\right\rangle\\
&= -2i\pi\delta\left(E_\alpha-E_\beta\right)V_{\beta\alpha}
\end{aligned} \tag{7.19}$$

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

$$\begin{aligned}
\left|\psi_\alpha^\pm\right\rangle &= \left|\psi_\alpha^0\right\rangle + G_0^\pm(E)V\left|\psi_\alpha^\pm\right\rangle\\
&= \left|\psi_\alpha^0\right\rangle + G^\pm(E)V\left|\psi_\alpha^0\right\rangle
\end{aligned} \tag{7.20a}$$

$$\begin{aligned}
S_{\beta\alpha} &= \left\langle\psi_\beta^-\middle|\psi_\alpha^+\right\rangle\\
&= \left\langle\psi_\beta^0\right| S\left|\psi_\alpha^0\right\rangle
\end{aligned} \tag{7.20b}$$

$\rightarrow$ exercise 3 sheet 8
or

$$\begin{aligned}
\left|\psi_\alpha^-\right\rangle - \left|\psi_\alpha^+\right\rangle &= G^-\\
&= \left(G^-(E_\alpha)-G^+(E_\alpha)\right)V\left|\psi_0^\alpha\right\rangle
\end{aligned} \tag{7.21a}$$

$$\left\langle\psi_\alpha^-\right| - \left\langle\psi_\alpha^+\right| = \left\langle\psi_\alpha^0\right| V\left(G^+(E_\alpha)-G^-\left(E_\alpha\right)\right) \tag{7.21b}$$

$$\begin{aligned}
S_{\beta\alpha} &= \left\langle\psi_\alpha^+\middle|\psi_\alpha^+\right\rangle\\
&= \left(\left\langle\psi_\beta^+\right| + \left\langle\psi_\beta^0\right| V\left(\frac{1}{E_\beta-H+i0^+}-\frac{1}{E_\beta-H-i0^+}\right)\right)\left|\psi_\alpha^+\right\rangle\\
&= \delta\left(\beta-\alpha\right) + \underbrace{\left(\frac{1}{E_\beta-E_\alpha+i0^+}-\frac{1}{E_\beta-E_\alpha-i0^+}\right)}_{\spadesuit}
\end{aligned} \tag{7.21c}$$

$$\begin{aligned}
\spadesuit: &\lim_{0+\searrow 0}\frac{-2i0^+}{\left(E_\beta-E_\alpha\right)^2+\left(0^+\right)^2}\\
&= -2i\pi\delta\left(E_\beta-E_\alpha\right)
\end{aligned} \tag{7.21d}$$

$$\delta(x) = \lim_{\varepsilon\searrow}\frac{1}{\pi}\frac{\varepsilon}{x^2+\varepsilon^2} \tag{7.21e}$$

Remark 7.2.1:

$$\begin{aligned}\sqrt{H}\left|\phi\right\rangle &= \sum \sqrt{E} c_\alpha \left|\psi_\alpha\right\rangle \\ &= \sum c_\alpha \sqrt{E_\alpha}\left|\psi_\alpha\right\rangle\end{aligned} \tag{7.22a}$$

with

$$\left|\phi\right\rangle = \sum c_\alpha \left|\psi_\alpha\right\rangle, \tag{7.22b}$$

$$H\left|\psi_\alpha\right\rangle = E_\alpha \left|\psi_\alpha\right\rangle, \tag{7.22c}$$

$$\Rightarrow \sqrt{H}\left|\psi_\alpha\right\rangle = \sqrt{E_\alpha}\left|\psi_\alpha\right\rangle. \tag{7.22d}$$

$$S_{\beta\alpha} = \delta(\beta-\alpha) - 2i\pi\delta(E_\alpha - E_\beta) \underbrace{\left\langle\psi_\beta^0\right| V \left|\psi_\alpha^+\right\rangle}_{T_{\beta\alpha}\ \text{transition matrix}} \tag{7.23a}$$

Chapter 8

Quantization of radiation field

8.1 Quantization of free radiation field

from section 5.1

$$\mathbf{A}(\mathbf{r},t) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_\lambda \left(\alpha(k\lambda)\, \boldsymbol{\epsilon}(k\lambda)\, e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} \right. \tag{8.1a}$$
$$\left. + \alpha^*(k,\lambda)\, \boldsymbol{\epsilon}^*(k,\lambda)\, e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega_k t} \right), \quad \omega = c|\mathbf{k}|$$

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

$$\mathbf{k}\cdot\boldsymbol{\epsilon}(k,\lambda) = 0 \tag{8.1b}$$

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

$$q_{k\lambda} = \alpha(k,\lambda)\, e^{-i\omega_k t} \tag{8.2a}$$

$$\ddot{q}_{k\lambda} = \omega_k^2 q_{k\lambda} \tag{8.2b}$$

$\to$ harmonics oscillator

Recall QMI: harmonic oscillator

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right) \tag{8.3a}$$

states

$$\hat{a}|0\rangle = 0 \tag{8.3b}$$

$$|n\rangle \equiv \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle \tag{8.3c}$$

The Hilbert space

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle \dots \tag{8.3d}$$

$$\hat{N} = \hat{a}^\dagger \hat{a} \tag{8.3e}$$

with

$$\hat{N}\,|n\rangle = n\,|n\rangle\,, \quad \text{etc.} \tag{8.3f}$$

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

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

$$H = \frac{1}{8\pi}\int \mathrm{d}^3\mathbf{r}\;\left(\mathbf{E}^2 + \mathbf{B}^2\right) \tag{8.4a}$$

$$\begin{aligned}\mathbf{E} &= -\frac{1}{c}\dot{\mathbf{A}} \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\sum_\lambda \left(\alpha\boldsymbol{\epsilon}\frac{i\omega}{c}e^{-i\omega t + i\mathbf{k}\cdot\mathbf{r}} - \alpha^*\boldsymbol{\epsilon}\frac{i\omega}{c}e^{i\omega t - i\mathbf{k}\mathbf{r}}\right)\end{aligned} \tag{8.4b}$$

$$\begin{aligned}\int \mathrm{d}^3\mathbf{r}\mathbf{E}^2 &= \int \mathrm{d}^3\mathbf{r}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\sum_{\lambda\lambda'}\left(\alpha\boldsymbol{\epsilon}e^{-i\omega t + i\mathbf{k}\mathbf{r}} - \alpha^*\boldsymbol{\epsilon}^*e^{i\omega t - i\mathbf{k}\mathbf{r}}\right)\left(\frac{i\omega}{c}\right) \\ &\quad\cdot\left(\alpha'\boldsymbol{\epsilon}'e^{i\omega' t + i\mathbf{k}'\cdot\mathbf{r}} - \alpha^{*\prime}\boldsymbol{\epsilon}^{*\prime}e^{i\omega' t - i\mathbf{k}'\cdot\mathbf{r}}\right)\left(\frac{i\omega'}{c}\right) \\ &= \int \mathrm{d}^3\mathbf{r}\iint\sum_{\lambda\lambda'}\left(\alpha\alpha'\boldsymbol{\epsilon}\times\boldsymbol{\epsilon}'^*\frac{-\omega\omega'}{c^2}e^{-it\left(\omega-\omega'\right)}e^{r\mathbf{r}\left(\mathbf{k}-\mathbf{k}'\right)}\right)\end{aligned} \tag{8.4c}$$

use

$$\int \mathrm{d}^3\mathbf{r}\;e^{i\mathbf{r}\left(\mathbf{k}-\mathbf{k}'\right)} = (2\pi)^3\,\delta\left(\mathbf{k}-\mathbf{k}'\right) \tag{8.4d}$$

$$\int \frac{\mathrm{d}^3k}{(2\pi)^3}\sum_{\lambda\lambda'}\left(\alpha\alpha'\boldsymbol{\epsilon}\times\boldsymbol{\epsilon}^{*\prime}\left(\frac{-\omega^2}{c^2}\right)+\dots\right) \tag{8.4e}$$

$$P = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\sum_\lambda \hbar\mathbf{k}a^*_{k\lambda}a_{k,\lambda} \tag{8.5a}$$

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

$$A.H, P \to \hat{A}, \hat{H}, \hat{P} \tag{8.6a}$$

commutation relations

$$\begin{aligned} \left[\hat{a}_{k\lambda}, \hat{a}_{k'\lambda'}\right] &= \left[\hat{a}^{!}_{k\lambda}, \hat{a}^{\dagger}_{k'\lambda'}\right] \\ &= 0 \end{aligned} \tag{8.6b}$$

$$\left[\hat{a}_{k\lambda}, \hat{a}^{\dagger}_{k'\lambda'}\right] = (2\pi)^3 \,\delta\left(k - k'\right) \delta_{\lambda\lambda'} \tag{8.6c}$$

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

λ**:** discrete

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

$$\begin{aligned} \mathcal{L} &= \frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu} \\ &= \frac{1}{8\pi}\left(E^2 - B^2\right) \end{aligned} \tag{8.7a}$$

define conjugate momentum field.

$$\begin{aligned} \pi &= \frac{\partial f}{\partial \mathbf{A}} \\ &= \dots \\ &= -\frac{1}{4\pi c}\mathbf{E}^2 \end{aligned} \tag{8.7b}$$

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

$$\begin{aligned} \left[A_i\left(x,t\right), A_j\left(y,t\right)\right] &= \left[\pi_i\left(x,t\right), \pi_j\left(y,t\right)\right] \\ &= 0 \end{aligned} \tag{8.8a}$$

$$\left[A_i, \pi_j\right] \approx i\hbar\delta\left(x - y\right)\delta_{ij} \tag{8.8b}$$

$$\begin{aligned} \mathbf{A}\left(\mathbf{r},t\right) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \sum_{\lambda} \Big(&\alpha\left(k,\lambda\right)\boldsymbol{\epsilon}\left(k,\lambda\right) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} \\ &+ \alpha^*\left(\mathbf{k},\lambda\right)\boldsymbol{\epsilon}^*\left(\mathbf{k},\lambda\right) e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega t}\Big) \end{aligned} \tag{8.9a}$$

$$H = \frac{1}{8\pi}\int \mathrm{d}^3\mathbf{r}\,\left(\mathbf{E}^2 + \mathbf{B}^2\right) \tag{8.9b}$$

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

use

$$\int \mathrm{d}^3 r\, e^{i(k\pm k')r} = (2\pi)^3\,\delta(k\pm k') \tag{8.9c}$$

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

$$\rightsquigarrow \int \mathrm{d}^3 v\,\mathbf{E}^2 = \frac{1}{(2\pi)^3}\int \mathrm{d}^3 k \left(-\frac{\omega^2}{c^2}\right)\big(\alpha_k\alpha_{-k}\boldsymbol{\epsilon}_k\boldsymbol{\epsilon}_{-k}e^{-2i\omega t} \tag{8.9d}$$
$$+\,\alpha_k^*\alpha_{-k}^*\boldsymbol{\epsilon}_k^*\boldsymbol{\epsilon}_k^* e^{2i\omega t} - \alpha_k\alpha_k^*\boldsymbol{\epsilon}_k\boldsymbol{\epsilon}_k^* - \alpha_k^*\alpha_{+k}\boldsymbol{\epsilon}_k^*\boldsymbol{\epsilon}_k\big)$$

$$\begin{aligned}\int \mathrm{d}^3\mathbf{r}\,\mathbf{B}^2 &= \dots \\ &= \int \frac{\mathrm{d}^3 k}{(2\pi)^3}\sum_\lambda \left(\frac{\omega^2}{c^2}\right)\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k - \{\cdots\}\right)\end{aligned} \tag{8.9e}$$

$$H = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\sum_\lambda \frac{\omega^2}{4\pi c^2}\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right) \tag{8.9f}$$

define:

$$\alpha^*(k,\lambda) = \sqrt{\frac{\omega}{2\pi c^2\hbar}}\alpha^*(k,\lambda) \tag{8.10a}$$

$$\mathbf{A}(\mathbf{r},t) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\sqrt{\frac{2\pi c^2\hbar}{\omega}}\sum_\lambda \left(q_{k\lambda}\boldsymbol{\epsilon}_{k\lambda}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + q^*_{k\lambda}\boldsymbol{\epsilon}^*_{k\lambda}e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\right) \tag{8.10b}$$

$$H = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\sum_\lambda \frac{\hbar\omega}{2}\left(a^*_{k\lambda}a_{k\lambda} + a_{k\lambda\lambda}a^*_{k\lambda}\right) \tag{8.10c}$$

$$\mathbf{P} = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\sum_\lambda \hbar\mathbf{k}a^*_{k\lambda}a_{k\lambda} \tag{8.10d}$$

8.1.1 2nd quantization

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

$$a(k,\lambda) \to \hat{a}(k,\lambda), \quad \text{operator} \tag{8.11a}$$

$$a^*(k,\lambda) \to \hat{a}^\dagger(k,\lambda), \quad \text{operator} \tag{8.11b}$$

as for harmonic oscillator

$$\mathbf{A}, H, \mathbf{P} \to \hat{\mathbf{A}}, \hat{H}, \hat{P} \tag{8.11c}$$

commutation relations:

$$\begin{aligned}\left[\hat{a}_{k\lambda}, \hat{a}_{k',\lambda'}\right] &= \left[\hat{a}^{k\lambda}_\dagger, \hat{a}^\dagger_{k',\lambda'}\right] \\ &= 0\end{aligned} \tag{8.12a}$$

$$\left[\hat{a}_{k\lambda}, \hat{a}^\dagger_{k'\lambda'}\right] = (2\pi)^3\delta\left(\mathbf{k}, -\mathbf{k}'\right)\delta_{\lambda\lambda'} \tag{8.12b}$$

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

λ: discrete, l.z

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

$$\begin{aligned}\mathcal{L} &= \frac{1}{16\pi}F_{\mu\nu}F^{\mu\nu} \\ &= \frac{1}{8\pi}\left(\mathbf{E}^2 - \mathbf{B}^2\right)\end{aligned} \tag{8.13a}$$

define conjugate momentum field

$$\begin{aligned}\pi &= \frac{\partial f}{\partial \mathbf{A}} \\ &= \dots \\ &= -\frac{1}{4\pi c}\mathbf{E}^2\end{aligned} \tag{8.13b}$$

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

$$\begin{aligned}\left[A_i\left(x,t\right), A_j\left(y,t\right)\right] &= \left[\pi_i\left(x,t\right), \pi_j\left(y,t\right)\right] \\ &= 0\end{aligned} \tag{8.13c}$$

$$\left[A_i, \pi_j\right] \approx i\hbar\delta\left(x-y\right)\delta_{ij} \tag{8.13d}$$

8.2 Fock space

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

$$\hat{a}^\dagger\left(k,\lambda\right) = \hat{a}^\dagger_{k\lambda}, \quad \text{creation operator} \tag{8.14a}$$

$$\hat{a}\left(k,\lambda\right) = \hat{a}_{k\lambda}, \quad \text{annihilation operator} \tag{8.14b}$$

start with vacuum $\left|0\right\rangle$ definition

$$\hat{a}_{k\lambda}\left|0\right\rangle = 0 \tag{8.14c}$$

$$\left|1\left(k,\lambda\right)\right\rangle = \hat{a}^\dagger\left|0\right\rangle \tag{8.14d}$$

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

General state

Note:

$$\begin{aligned}&\hat{a}^\dagger_{k_j\lambda_j}\left|n_1\left(k_1,\lambda_1\right)\dots n_j\left(k_j,\lambda_j\right)\dots n_m\left(k_m,\lambda_m\right)\right\rangle \\ &\quad = \sqrt{n_j+1}\left|n_1\dots n_{j+1}\dots n_m\right\rangle\end{aligned} \tag{8.15a}$$

$$\int\frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3}\sum_\lambda \hat{a}_{k\lambda}\left|n_1\left(k_1,\lambda_1\right)\right\rangle = \frac{1}{\sqrt{n_1!}}\int\frac{\mathrm{d}^3k}{\left(2\pi\right)^3}\sum_\lambda \hat{a}_{k\lambda}\left(\hat{a}^\dagger_{k_1\lambda_1}\right)^{n_1}\left|0\right\rangle \tag{8.15b}$$

with

$$\hat{a}_{k\lambda}\left(\hat{a}^\dagger_{k_1\lambda_1}\right)^{n_1}\left|0\right\rangle = \left(\hat{a}^\dagger_{k_1\lambda_1}\right)^{n_1-1}n_1\left[\hat{a}_{k\lambda}, \hat{a}^\dagger_{k_1\lambda_1}\right] + \left(\hat{a}^\dagger_{k_1\lambda_1}\right)\hat{a}_{k\lambda} \tag{8.15c}$$

with

$$\left[\hat{a}_{k\lambda}, \hat{a}^{\dagger}_{k_1\lambda_1}\right] = n_1 \left(2\pi\right)^3 \delta\left(\mathbf{k} - \mathbf{k}_1\right) \delta_{\lambda\lambda_1} \tag{8.15d}$$

$$\begin{aligned}
\rightsquigarrow \int \frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3} \sum_{\lambda} \hat{a}_{k\lambda} \left|n_1\left(k_1, \lambda_1\right)\right\rangle &= \frac{n_1}{\sqrt{n_1!}} \left({}^{\dagger}_{k_1\lambda_1}\right)^{n_1-1} \left|0\right\rangle \\
&= \frac{n_1\sqrt{\left(n_1-1\right)!}}{\sqrt{n_1!}} \frac{\left(\hat{a}^{\dagger}_{k_1\lambda_1}\right)^{n_1-1}}{\sqrt{\left(n_1-1\right)!}} \left|0\right\rangle \\
&= \sqrt{n_1} \left|\left(n_1-1\right)\left(k_1\lambda_1\right)\right\rangle
\end{aligned} \tag{8.15e}$$

General:

$$\int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3} \sum_{\lambda} a_{k\lambda} \left|n_1 \dots n_m\right\rangle = \sum_{i=1}^{m} \sqrt{n_i} \left|n_1 \dots n_{i-1}, \dots n_m\right\rangle \tag{8.16a}$$

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

$$\left\langle n_1\right| \hat{H} \left|n_1\right\rangle = \int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3} \sum_{\lambda} \frac{\hbar\omega}{2} \left\langle n_1\right| \hat{a}^{\dagger}_{k\lambda}\hat{a}_{k\lambda} + \underbrace{\hat{a}_{k\lambda}\hat{a}^{\dagger}_{k\lambda}}_{\hat{a}^{\dagger}_{k\lambda}\hat{a}_{k\lambda}} + \delta(0) \left|n_1\right\rangle \tag{8.16b}$$

$$\begin{aligned}
\left\langle n_1\right| \hat{H} \left|n_1\right\rangle &= \int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3} \sum_{\lambda} \hbar\omega \left\langle n_1\right| \hat{a}^{\dagger}_{k\lambda}\hat{a}_{k\lambda} \left|n_1\right\rangle \\
&= \hbar\omega \left\langle n_1\right| \hat{a}^{\dagger}_{k_1\lambda_1} \left|n_1 - 1\right\rangle \sqrt{n_1} \\
&= \hbar\omega n_1 \left\langle n_1 \middle| n_1\right\rangle \\
&= n_1\hbar\omega
\end{aligned} \tag{8.16c}$$

$$\to \left\langle n_1 \dots n_m\right| \hat{H} \left|n_1 \dots n_m\right\rangle = \sum_{i=1}^{m} \hbar\omega_i n_i \tag{8.16d}$$

introduce interactions with matter (compare Section 5)

$$V = -\frac{q}{2mc}\left(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}\right) + \frac{q^2}{2mc^2}\hat{\mathbf{A}}^2 \tag{8.17a}$$

in Coulomb gauge

$$\boldsymbol{\nabla}\cdot\mathbf{A} = 0 \tag{8.18a}$$

$$\Rightarrow \mathbf{p}\cdot\mathbf{A} = \mathbf{A}\cdot\mathbf{p} \tag{8.18b}$$

$$\hat{V} = -\frac{q_-}{mc} p\cdot\hat{A} + \frac{q^2}{2mc^2}\hat{A}^2 \tag{8.18c}$$

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

$$V_{\beta\alpha} = \left\langle \psi_\beta^0 \right| V \left| \psi_\alpha^0 \right\rangle \tag{8.18d}$$

8.3 Photon emission and absorption

We have considered these processes before in section 5.2

$$\begin{aligned} H &= H_0 + H_{\text{em}} + \hat{V} \\ &= \sum_i \frac{p_i^2}{2m} + \frac{1}{8\pi} \int \mathrm{d}^3 r \left(\hat{\mathbf{E}}^2 + \hat{\mathbf{B}}^2 \right) \\ &\quad + \text{interaction matter} \leftrightarrow \text{photons} \end{aligned} \tag{8.19a}$$

$$\begin{aligned} \text{eigenstates } \left| \psi_\alpha^0 \right\rangle &= |\text{matter}\rangle \otimes |\text{photons}\rangle \\ &= \text{wave function} \otimes \text{new, Fockspace} \\ &= |A; n_1 (k, \lambda_1) \dots n_m (k_m, \lambda_m)\rangle \end{aligned} \tag{8.19b}$$

8.3.1 Absorption of photon

$$V_{\beta\alpha} = \langle B; (n-1)(k,\lambda) | \hat{V} | A; n(k,\lambda) \rangle \tag{8.20a}$$

with

B**:** final state of atom

$(n-1)$**:** one photon "lost"

A**:** initial state of atom

$n(k,\lambda)$**:** n photons, k, λ

$$\begin{aligned} \rightsquigarrow V_{\beta\alpha} &= \frac{e}{mc} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{\lambda'} \sqrt{\frac{2\pi\hbar c^2}{\omega'}} \\ &\quad \cdot \langle B; (n-1)(k,\lambda) | \hat{a}(k',\lambda') \, \mathbf{p} \cdot \boldsymbol{\epsilon}(k',\lambda') \, e^{i\mathbf{k}'\cdot\mathbf{r}} | A, n(k,\lambda) \rangle \end{aligned} \tag{8.20b}$$

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

$$\begin{aligned} \rightsquigarrow V_{\beta\alpha} &= \frac{e}{m} \sqrt{\frac{2\pi\hbar}{\omega}} \sqrt{n} \, \langle B; | \, \mathbf{p} \cdot \boldsymbol{\epsilon}(k,\lambda) e^{i\mathbf{k}\cdot\mathbf{r}} \, |A\rangle \\ &\sim \sqrt{n} \end{aligned} \tag{8.20c}$$

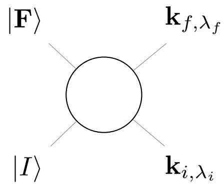

Figure 8.1:

8.3.2 Emission of photons

$$V_{\beta\alpha} = \langle B; (n+1)(k,\lambda)| \hat{V} |A; n(k,\lambda)\rangle, \tag{8.21a}$$

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

$$\begin{aligned} \rightsquigarrow V_{\beta\alpha} &= \frac{e}{m}\sqrt{\frac{2\pi\hbar}{\omega}}\sqrt{n+1}\langle B| \mathbf{p}\cdot\boldsymbol{\epsilon}^*(k,\lambda)\, e^{-i\mathbf{k}\cdot\mathbf{r}}|A\rangle \\ &\sim \sqrt{n+1} \end{aligned} \tag{8.21b}$$

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

$$\Gamma_{n0} = \Gamma_{0n} \tag{8.22a}$$

$$\text{absorption} = \text{emission} \tag{8.22b}$$

now

$$\frac{\Gamma_{n0}}{\Gamma_{0n}} = \frac{n_{k\lambda}}{n_{k\lambda}+1} \tag{8.22c}$$

8.4 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

$$\hat{V} = \frac{e}{mc}\mathbf{p}\cdot\hat{\mathbf{A}} + \frac{e^2}{2mc^2}\hat{\mathbf{A}}^2 \tag{8.23}$$

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

first-order contribution

$$
\begin{aligned}
V_{\beta\alpha}^{(1)} &= \langle F, 1\left(k_f, \lambda_f\right)| \frac{e^2}{2mc^2} \hat{\mathbf{A}}^2 \left|I, 1\left(k_i, f_i\right)\right\rangle \\
&= \frac{e^2}{2mc^2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3} \sum_{\lambda\lambda'} \frac{2\pi\hbar c^2}{\sqrt{\omega\omega'}} \\
&\quad \cdot \langle F, 1\left(k_f, \lambda_f\right)| \left(\hat{a}\boldsymbol{\epsilon} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + \hat{a}^\dagger\left(k,\lambda\right) e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\right) \\
&\quad \cdot \left(\hat{a}'\left(k',\lambda'\right) e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + \hat{a}^{\dagger\prime} \boldsymbol{\epsilon}'^* e^{-i\mathbf{k}\cdot\mathbf{r}+i'wt}\right) \left|I, 1\left(k_i, \lambda_i\right)\right\rangle \\
&= \frac{e^2}{2mc^2} \frac{2\pi\hbar c^2}{\sqrt{\omega_i\omega_f}} 2 \cdot \langle F| \boldsymbol{\epsilon}\left(k_i, \lambda_i \cdot \boldsymbol{\epsilon}\left(k_f, \lambda_f\right) e^{it\left(\omega_i-\omega_f\right)}\right) e^{i\mathbf{r}\cdot\left(\mathbf{k}_i-\mathbf{k}_f\right)} \left|I\right\rangle
\end{aligned}
\tag{8.24}
$$

Recall from section 7.2

$$H = H_0 + V \tag{8.25a}$$

$$
\begin{aligned}
S_{\beta\alpha} &= \delta\left(\beta-\alpha\right) - \frac{i}{\hbar} \int_{\mathbb{R}} \mathrm{d}t_1 \, e^{-\frac{i}{\hbar}t_1\left(E_\alpha - E_\beta\right)} \left\langle \psi_\beta^0 \right| V \left|\psi_\alpha^0\right\rangle \\
&\quad - \frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t_1 \, e^{-\frac{i}{\hbar}t_1\left(E_I + \hbar\omega_i - E_F - \hbar\omega_f\right)} \left(\frac{2e^2\hbar\pi}{m\sqrt{\omega_i\omega_f}} \boldsymbol{\epsilon} \right. \\
&\qquad \left. \cdot \boldsymbol{\epsilon}^* \left\langle F \right| \ldots \left| F \right\rangle \right)
\end{aligned}
\tag{8.25b}
$$

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

$$
\begin{aligned}
\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} &= \frac{k^2 \, \mathrm{d}k \, \mathrm{d}\Omega}{(2\pi)^3} \\
&= \frac{\omega_f^2 \, \mathrm{d}\Omega}{(2\pi)^3 c^3 \hbar} \mathrm{d}(\hbar\omega_f)
\end{aligned}
\tag{8.26a}
$$

$$\rho\left(\omega_f\right) = \frac{\omega_f^2 \, \mathrm{d}\Omega}{(2\pi)^3 c^3 \hbar} \tag{8.26b}$$

Feynman diagrams

Figure 8.2:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{c}\frac{2\pi}{\hbar}\underbrace{\frac{\omega_f^2}{(2\pi)^3 c^3\hbar}}_{\rho(\omega_f)}|T|^2 \tag{8.27a}$$

$$= \frac{e^4}{m^2c^4}\frac{\omega_f}{\omega_i}\left|\boldsymbol{\epsilon}_i\cdot\boldsymbol{\epsilon}_f^*\langle F|\, e^{i\mathbf{r}\cdot(\mathbf{k}_i-\mathbf{k}_f)}\,|I\rangle\right|^2$$

$$\left(\frac{\alpha\hbar}{mc}\right)^2 = r_0^2 \tag{8.27b}$$

(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)...

2nd order contribution for $T_{\beta\alpha}$

$$S_{\beta\alpha} = \ldots\left(-\frac{i}{\hbar}\right)^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\sum_\gamma e^{-\frac{i}{\hbar}t_1(E_\gamma-E_\beta)}e^{-\frac{i}{\hbar}t_2(E_\alpha-E_\gamma)}V_{\beta\gamma}V_{\gamma\alpha} \tag{8.28a}$$

In our case

$$\left(-\frac{i}{\hbar}\right)^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2 \sum\!\!\!\!\!\!\int \mathrm{d}N\, e^{-\frac{i}{\hbar}(E_N-E_F)t_i}e^{-\frac{i}{\hbar}(E_I-E_N)t_2}\left(\frac{e}{mc}\right)^2$$
$$\cdot\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\sum_{\lambda\lambda'}\langle F, P(\omega_f,\lambda_f)|\,\hat{a}_k\mathbf{p}\cdot\boldsymbol{\epsilon}_k e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t_1+\hat{a}_k^\dagger\mathbf{p}\cdot\boldsymbol{\epsilon}_k^* e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t_1}}\,|N\rangle$$
$$\cdot\langle N|\,\hat{a}_{k'}\mathbf{p}\cdot\boldsymbol{\epsilon}_{k'}e^{i\mathbf{k}'\cdot\mathbf{r}-i\omega' t_2}+\hat{a}_{k'}^\dagger\mathbf{p}\cdot\boldsymbol{\epsilon}_{k'}^* e^{-i\mathbf{k}'j\mathbf{r}+i\omega' t_2}\,|I, 1(k_i,\lambda_i)\rangle \tag{8.29a}$$

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

$$\begin{aligned}&= \ldots\\ &= \langle F|\,\hat{a}_{k_f}^\dagger\ldots|N\rangle\langle N|\ldots\hat{a}_{k_i}|I\rangle+\langle F|\,\hat{a}_{k_i}\ldots|N\rangle\langle N|\ldots\hat{a}_\dagger^{k_f}\,|I\rangle\end{aligned} \tag{8.29b}$$

Kramers Heisenberg formula

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{\alpha\hbar}{mc}\right)^2 \frac{\omega_f}{\omega_i} \Bigg| \boldsymbol{\epsilon}_i \boldsymbol{\epsilon}_f^* \delta_{FI} + \sum_N \langle F| \mathbf{p}\cdot\boldsymbol{\epsilon}_f^* |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}_i |I\rangle + \frac{\langle F| \mathbf{p}\cdot\boldsymbol{\epsilon}_i |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}_f^* |I\rangle}{m\left(E_I - \hbar\omega_f - E_N\right)} \Bigg| \tag{8.30}$$

$\to$ limiting cases

Rayleight scattering elastic scattering

$$|I\rangle = |F\rangle\,, \tag{8.31a}$$

$$\omega_i = \omega_f \tag{8.31b}$$

$$\hbar\omega \ll E_I - E_N \tag{8.31c}$$

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

$$\begin{aligned}\langle I| \boldsymbol{\epsilon}_i \boldsymbol{\epsilon}_f^* |I\rangle &= \frac{1}{i\hbar} \langle I| \left[\mathbf{x}\cdot\boldsymbol{\epsilon}_i, \mathbf{p}\cdot\boldsymbol{\epsilon}_f^*\right] |I\rangle \\ &= \frac{1}{i\hbar} \sum_N \big(\langle I| \mathbf{x}\cdot\boldsymbol{\epsilon}_i |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}_f^* |I\rangle \\ &\qquad - \langle I| \mathbf{p}\cdot\boldsymbol{\epsilon}_f^* |N\rangle \langle N| \mathbf{p}\cdot\boldsymbol{\epsilon}_f^* |I\rangle \big)\end{aligned} \tag{8.32a}$$

$\to$ put everything together:

$$\frac{1}{E_N - E_I} + \frac{1}{E_I - E_N + \pm\hbar\omega} = \mp\frac{\hbar\omega}{\left(E_I - E_N\right)^2} + \frac{\left(\hbar\omega\right)^2}{\left(E_I - E_N\right)^2} + \dots \tag{8.33a}$$

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

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

$$\hbar\omega_i \gg E_N - E_I \tag{8.34a}$$

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

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = r^2 \left|\boldsymbol{\epsilon}_i \cdot \boldsymbol{\epsilon}_f\right|^2 \tag{8.34b}$$

for unpolarized photons

$$\begin{aligned}
&\frac{1}{2}\sum_{\lambda_i\lambda_f} \varepsilon_i^a\left(k_i,\lambda_i\right)\left(\varepsilon_f\right)^a\left(k_f,\lambda_f\right)\varepsilon_i^b\left(\varepsilon_f^*\right)^b \\
&\quad=\frac{1}{2}\left(\delta_{ab}-\frac{k_i^a k_i^b}{k_i^)}\right)\left(\delta_{ab}-\frac{k_f^a k_f^b}{k_f^2}\right) \\
&\quad=\frac{1}{2}\left(1+\cos^2\theta\right)
\end{aligned} \tag{8.34c}$$

with

$$\theta=\sphericalangle\left(\mathbf{k}_i,\mathbf{k}_f\right) \tag{8.34d}$$

$$\begin{aligned}
\sigma &= \int \mathrm{d}\cos\theta\, 2\pi r_0^2\left(1+\cos^2\theta\right) \\
&= \frac{8\pi}{3} r_0^2
\end{aligned} \tag{8.34e}$$

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

$$e^{-\frac{i}{\hbar}E_N t}e^{-\tau_N t}=e^{-\frac{i}{\hbar}t\left(E_N-i\Gamma_N\right)} \tag{8.35a}$$

with Γ_N that one cannot neglect

$$\begin{aligned}
|T|^2 &\approx \left|\frac{1}{E_I-E_N+i\Gamma_N}\right|^2 \\
&= \frac{1}{\left(E_I-E_N\right)^2+\Gamma_N^2}
\end{aligned} \tag{8.35b}$$

Chapter 9

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

9.1 Klein-Gordon equation (KGE)

Consider dfree scalar particle

$$\begin{aligned} X^{\mu} &\rightarrow X^{\mu'} \\ &= \Lambda^{\mu}_{\ \nu} x^{\nu} \end{aligned} \tag{9.1a}$$

$$\begin{aligned} \phi(x) &\rightarrow \phi'\left(x'\right) \\ &= \phi(x) \\ &= \phi\left(\Lambda^{-1} x'\right) \end{aligned} \tag{9.1b}$$

Now start from

$$E^2 = m^2 c^4 + \mathbf{p}^2 c^2 \tag{9.2a}$$

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

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \tag{9.2b}$$

$$\mathbf{p} = -i\hbar \boldsymbol{\nabla} \tag{9.2c}$$

$$\left(-\hbar^2 \frac{\partial^2}{\partial t^2}\right) \phi(\mathbf{x}, t) = \left(m^2 c^4 - \hbar c^2 \boldsymbol{\nabla}^2\right) \phi(x, t) \tag{9.2d}$$

in covariant form:

$$\partial_\mu \partial^\mu + \frac{m^2c^2}{\hbar^2}\phi(x) = 0 \tag{9.2e}$$

$$\begin{aligned}\partial_\mu &= \frac{\partial}{\partial x^\mu} \\ &= \left(\frac{1}{c}\frac{\partial}{\partial t}, \boldsymbol{\nabla}\right)\end{aligned} \tag{9.2f}$$

$$\partial^\mu = \left(\frac{1}{c}\frac{\partial}{\partial t} - \boldsymbol{\nabla}\right) \tag{9.2g}$$

KGE:

$$\left(\partial_\mu \partial^\mu + \frac{m^2c^2}{\hbar^2}\right)\phi = 0 \tag{9.3a}$$

$$\partial_\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, \boldsymbol{\nabla}\right) \tag{9.3b}$$

Solution

$$\phi\left(t, \mathbf{x}\right) = A \cdot e^{i\mathbf{k}\cdot\mathbf{x} - i\omega t} \tag{9.3c}$$

$$\phi(x) = A \cdot e^{-ik_\mu x^\mu} \tag{9.3d}$$

$$k^\mu = \left(\frac{\omega}{c}, \mathbf{k}\right), \quad k^2 = k_\mu k^\mu = \frac{\omega^2}{c^2} - \mathbf{k}^2 = \frac{m^2c^2}{\hbar^2} \tag{9.3e}$$

or

$$(h\omega) = \pm\sqrt{m^2c^4 + \mathbf{p}^2c^2} \tag{9.3f}$$

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

$$\frac{\partial}{\partial t}\rho + \boldsymbol{\nabla}\mathbf{j} = 0 \tag{9.4a}$$

$$\mathbf{j} = \frac{\hbar}{2mi}\left(\phi^*\left(\nabla\phi\right) - \left(\nabla\phi^*\right)\phi\right) \tag{9.4b}$$

$$\rho = \frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial t} - \frac{\partial\phi^*}{\partial t}\phi\right) \tag{9.4c}$$

covariant form

$$\begin{aligned}j^\mu &= (cp, j) \\ &= \frac{i\hbar}{2m}\left(\phi^*\partial^\mu\phi - \left(\partial^\mu\phi^*\right)\phi\right)\end{aligned} \tag{9.4d}$$

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

9.2 Dirac equation

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

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t}\psi &= H\psi \\
&= \left(-i\hbar c\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2\right)\psi \\
&= \left(-i\hbar c\alpha_i\nabla_i + \beta mc^2\right)\psi
\end{aligned}
\tag{9.5a}
$$

With summation convention and

$$
\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3) \tag{9.5b}
$$

and β are 4 non-commeting coefficients

Iterate tis equation

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

Compare to KGE

$$
-\hbar^2 \frac{\partial^2}{\partial t^2}\psi = \left(-\hbar c^2\nabla_i\nabla_i + m^2c^4\right)\psi \tag{9.6a}
$$

$$
\beta^2 = 1 \tag{9.6b}
$$

$$
\begin{aligned}
(\alpha_i\beta + \beta\alpha_i) &= \{\alpha_i, \beta\} \\
&= 0, \quad (\text{sometimes } [\alpha_i, \beta]_+)
\end{aligned}
\tag{9.6c}
$$

$$
\begin{aligned}
(\alpha_i\alpha_j + \alpha_j\alpha_i) &= \{\alpha_i, \alpha_j\} \\
&= 2\delta_{ij}
\end{aligned}
\tag{9.6d}
$$

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

$$
\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \tag{9.7}
$$

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

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \tag{9.8a}$$

$$\begin{aligned} \beta &= \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \text{Dirac representiation} \end{aligned} \tag{9.8b}$$

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

$$\gamma^\mu, \quad \mu \in \{0,1,2,3\}, \gamma^0 = \beta, \gamma^i = \beta\alpha^i \tag{9.9a}$$

in Dirac representation

$$\gamma^0 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \tag{9.9b}$$

$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \tag{9.9c}$$

Note cane use any other representation:

$$\gamma^\mu \to U\gamma^\mu U^{‘]} \tag{9.10a}$$

Take β: Dirac equation

$$\beta \cdot \left(i\hbar\frac{\partial}{\partial t}\right)\psi = \beta\left(-i\hbar c\alpha_i\nabla_i + \beta mc^2\right)\psi \tag{9.10b}$$

$$i\hbar\frac{\partial}{\partial t}\gamma^0\psi = \left(-i\hbar c\gamma^i\nabla_i + mc^2\right)\psi \tag{9.10c}$$

$$\left(i\hbar\partial_\mu - mc\right)\psi = 0 \tag{9.10d}$$

Notation any 4-vector a^μ:

$$\not{\partial} \equiv a_\mu\gamma^\mu \tag{9.10e}$$

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

$$\left(i\hbar \not{\partial} - mc\right)\psi = 0 \tag{9.10f}$$

Properties of γ matrices:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \tag{9.10g}$$

$$\gamma^0\gamma^\mu\gamma^0 = (\gamma^\mu)^\dagger \tag{9.10h}$$

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

$$\begin{aligned} \left(i\hbar\partial_\mu\gamma^\mu - mc\right)\psi &\equiv \left(i\hbar\partial\!\!\!/ - mc\right)\psi \\ &= 0 \end{aligned} \tag{9.11a}$$

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\,\mathrm{Id} \tag{9.11b}$$

The adjoint Dirac equation

$$\begin{aligned} 0 &= \gamma^+ \left(i\hbar\partial_\mu \left(\gamma^\mu\right)^\dagger - mc\right) \\ &= \psi^\dagger \left(-i\hbar \overleftarrow{\partial}_\mu \gamma^0\gamma^\mu\gamma^0 - \gamma^0\gamma^0 - \gamma^0\gamma^0 mc\right) \\ &= \psi^\dagger\gamma^0 \left(\overleftarrow{\partial}_\mu - mc\right)\gamma^0 \\ &= 0 \end{aligned} \tag{9.11c}$$

$$\Rightarrow \overline{\psi}\left(i\hbar\partial\!\!\!/ + mc\right) = 0 \tag{9.11d}$$

$$\overline{\psi} \equiv \psi^\dagger\gamma^0 \tag{9.11e}$$

The current:

$$j^\mu \equiv \overline{\psi}\gamma^\mu\psi \tag{9.12a}$$

$$\begin{aligned} \partial_\mu j^\mu &= \left(\partial\!\!\!/\overline{\psi}\right)\psi + \overline{\psi}\partial\!\!\!/\psi \\ &= 0 \end{aligned} \tag{9.12b}$$

$$\begin{aligned} \rho &\equiv j^0 \\ &= \psi^\dagger\gamma^0\gamma^0\psi \\ &= \psi^\dagger\psi, \quad \text{positive definite} \end{aligned} \tag{9.12c}$$

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

9.3 Coraviance of Dirac equation

Consider LT

$$\begin{aligned} x^\mu &\rightarrow x'^\mu \\ &= \Lambda^\mu{}_\nu x^\nu \\ &= \frac{\partial x'^\mu}{\partial x^\nu} x^\nu, \quad (x \rightarrow \Lambda x) \end{aligned} \tag{9.13a}$$

Dirac

$$\left(i\hbar\partial_\mu\gamma^\mu - mc\right)\psi(x) = 0 \tag{9.13b}$$

$$\rightarrow \left(i\hbar\partial'_\mu - mc\right)\psi\left(x'\right) = 0 \tag{9.13c}$$

require transformation

$$\begin{aligned}\psi(x) &\rightarrow \psi'(x') \\ &= S\,(\Lambda)\,\psi(x)\end{aligned} \tag{9.13d}$$

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

$$\begin{aligned}S(\Lambda)\left(i\hbar\frac{\partial}{\partial x^\mu}\gamma^\mu - mc\right)\psi &= S\,(\Lambda)\,(i\hbar\Lambda^\nu{}_\mu\partial'_\nu\gamma^\mu - mc)\,\psi \\ &= S(\Lambda)\,(i\hbar\Lambda^\nu{}_\mu\partial'_\nu\gamma^\mu - mc)\,\psi \\ &= \big(i\hbar S(\Lambda)\,(\Lambda^\nu{}_\mu\gamma^\mu)\,S^{-1}\,(\Lambda)\,\partial'_\nu \\ &\qquad - mc\big)\,\underbrace{S(\Lambda)\psi(x)}_{\psi'(x')}\end{aligned} \tag{9.13e}$$

Compare with Dirac in S'

$$S(\Lambda)\Lambda^\nu{}_\mu\gamma^\mu S^{-1}(\Lambda) = \gamma^\nu \tag{9.13f}$$

or

$$\Lambda^\nu{}_\mu\gamma^\mu = S^{-1}(\Lambda)\gamma^\nu S(\Lambda) \tag{9.13g}$$

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

$$\omega_{\rho\sigma} = -\omega_{\sigma\rho}, \quad \text{(antisymmetric)} \tag{9.13h}$$

Claim: For infinitesimal propel LT:

$$S(\Lambda) = \mathbf{1} + \frac{i}{2}\omega_{\mu\nu}\sigma^{\mu\nu} \tag{9.14a}$$

with

$$\sigma^{\mu\nu} \equiv \frac{i}{2}\,[\gamma^\mu, \gamma^\nu] \tag{9.14b}$$

or for finite LT

$$S(\Lambda) = e^{\frac{i}{2}\omega_{\mu\nu}\sigma^{\mu\nu}} \tag{9.14c}$$

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

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

$$\Lambda^\mu{}_\nu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{9.15a}$$

we get for $\nu = 0$

$$S\gamma^0 S = \gamma^0 \tag{9.15b}$$

and for $\nu = i$

$$S\gamma^i S = -\gamma^i \tag{9.15c}$$

$$S\left(\Lambda_p\right) = \gamma^0 \times \underbrace{\text{Phase}}_{1} \tag{9.15d}$$

Define

$$\gamma_5 \equiv i\gamma_0\psi_1\gamma_2\psi_3 \tag{9.16a}$$

in Dirac representation

$$\gamma_5 = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \tag{9.16b}$$

Note

$$(\gamma_5) = \mathbf{1}\,. \tag{9.16c}$$

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

$$\psi(x) \xrightarrow{\text{LT}} S(\Lambda)\psi(x) \tag{9.17a}$$

$$\overline{\psi}(x) \xrightarrow{\text{LT}} \overline{\psi}(x)S^{-1}(\Lambda) \tag{9.17b}$$

$\rightarrow$ exercise sheet 12

9.3.1 Bilinear covariants

$$\overline{\psi}(x)\psi(x) \xrightarrow{\text{pLT}} \overline{\psi}S^{-1}S\psi = \overline{\psi}(x)\psi(x) \tag{9.18a}$$

$$\xrightarrow{\text{Parity}} \overline{\psi}\gamma^0\gamma^0\psi = \overline{\psi}(x)\psi(x) \tag{9.18b}$$

$$\overline{\psi}(x)\gamma_5(x)\psi(x) \xrightarrow{\text{pLT}} \overline{\psi}S^{-1}\gamma^5 S\psi = \overline{\psi}\gamma_5\psi \tag{9.18c}$$

$$\left\{\gamma^5, \gamma^\mu\right\} = 0 \tag{9.18d}$$

$$\Rightarrow [S, \gamma_5] = 0 \tag{9.18e}$$

$$\overline{\psi}\gamma^\mu\psi \rightarrow \Lambda^\mu{}_\nu\overline{\psi}\gamma^\nu\psi, \quad \text{vector} \tag{9.19a}$$

$$\overline{\psi}\gamma_5\gamma^\mu\psi \rightarrow \text{Det}(\Lambda)\Lambda^\mu{}_\nu\overline{\psi}\gamma^\nu\gamma_5\psi, \quad \text{axial vector} \tag{9.19b}$$

$$\overline{\psi}\sigma^{\mu\nu}\psi \rightarrow \Lambda^\mu{}_\rho\Lambda^\nu{}_\sigma\overline{\psi}\gamma^{\rho\sigma}\psi, \quad \text{tensor rank 2} \tag{9.19c}$$

9.4 Solutions to the dirac equation

$$\psi(x) = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \tag{9.20}$$

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

$$\psi^+(x) = e^{-ikx}u(k), \quad \text{positive } E \tag{9.21a}$$
$$\psi^-(x) = e^{ikx}v(k), \quad \text{negative } E \tag{9.21b}$$

$$\begin{aligned} \mathbf{k}\cdot\mathbf{x} &= k_\mu x^\mu \\ &= \omega t - \mathbf{x}\cdot\mathbf{k} \end{aligned} \tag{9.22a}$$

write as:

$$\psi^+ = e^{-\frac{i}{\hbar}(Et-px)}u(p) \tag{9.22b}$$
$$\psi^- = e^{\frac{i}{\hbar}(-Et-px)}u(p) \tag{9.22c}$$
$$p^\mu = \left(\frac{E}{c}, p\right) \tag{9.22d}$$

Dirac

$$(\not{p} - mc)\, u(p) = 0 \tag{9.23a}$$
$$-\not{p} - mcv(p) = 0 \tag{9.23b}$$

are matrix equations

$$\begin{aligned}(\not{p} \mp mc) &= \begin{pmatrix} \frac{E}{c} \mp mc & -\mathbf{p}\cdot\boldsymbol{\sigma} \\ \mathbf{p}\cdot\boldsymbol{\sigma} & -\frac{E}{c} \mp mc \end{pmatrix} \begin{pmatrix} \chi \\ \varphi \end{pmatrix} \\ &= 0 \end{aligned} \tag{9.23c}$$

par. of u and/or v

$$u(p) \equiv \begin{pmatrix} \chi \\ \varphi \end{pmatrix} \tag{9.23d}$$

$$\varphi = \left(\frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{E + mc^2}\right)\chi \tag{9.23e}$$

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

$$u\left(p,r\right)=\begin{pmatrix}\sqrt{E+mc^2} & \chi_r \\ \frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{\sqrt{E+mc^2}}\chi_r\end{pmatrix} \tag{9.23f}$$

and

$$v(p,r)=\begin{pmatrix}\frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{\sqrt{E+mc^2}} & \chi_r \\ \sqrt{E+mc^2} & \chi_r\end{pmatrix} \tag{9.23g}$$

$$\chi_1=\begin{pmatrix}1\\0\end{pmatrix} \tag{9.23h}$$

$$\chi_2=\begin{pmatrix}0\\1\end{pmatrix} \tag{9.23i}$$

r related to spin, 4-solutions

some propertes of u and v:

$$\overline{u}\left(p,r_i\right)u\left(p,r_j\right)=u^\dagger\left(p,r_i\right)\gamma^0 u\left(p,R-j\right) \tag{9.23j}$$

$$\begin{aligned}&\begin{pmatrix}\sqrt{E+mc^2}\chi_i & \frac{c\mathbf{p}\cdot\boldsymbol{\sigma}}{\sqrt{E+mc^2}\chi_i}\cdot\end{pmatrix}\begin{pmatrix}\mathbf{1} & 0\\ 0 & -\mathbf{1}\end{pmatrix}\begin{pmatrix}\sqrt{E+mc^2} & \chi_j\\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{\sqrt{E+mc^2}} & \chi_j\end{pmatrix}\\ &\quad=\left(\left(E+mc^2\right)\chi_i\cdot\chi_j-\frac{c\mathbf{p}^2}{\left(Emc^2\right)}\chi_i\chi_j\right.\\ &\quad=2mc^2\chi_i\chi_j\\ &\quad=2mc^2\delta_{ij}\end{aligned} \tag{9.23k}$$

similar

$$\overline{v}\left(p,r_i\right)v\left(p,r_j\right)=-2mc^2\delta_{ij} \tag{9.23l}$$

and

$$\begin{aligned}\overline{v}u&=\overline{u}v\\ &=0\end{aligned} \tag{9.23m}$$

Convention: In some books

$$u/v\to\frac{1}{\sqrt{2mc^2}}u/v \tag{9.23n}$$

$\rightarrow u,v$ form a basis

We can also show:

$$\sum_{i\ =1}^{3}u\left(p,r_i\right)\cdot\overline{u}\left(p,r_i\right)=c\left(\not{p}+mc\right) \tag{9.24a}$$

$\leftarrow$ projection to positios energy states

$$\sum v(p, r_i) \cdot \overline{v}(p, r_i) = c(-\not{p} + mc) \tag{9.24b}$$

$\leftarrow$ negative

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

$$\left(\sum_{i=1}^{3} u(p, r_i) \cdot \overline{u}(p, r_i)\right) u(p, r_j) = 2mc^2 u(p, r_j) \ldots \tag{9.24c}$$

9.4.1 Interpretation of solutions and spin

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

$$H = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc^2 \tag{9.25a}$$

$$\mathbf{L} = \mathbf{x} \times \mathbf{p} \tag{9.25b}$$

$$\begin{aligned} [L_i, H] &= [\varepsilon_{ijk} x_j p_k, \alpha_\ell p_\ell] \\ &= \varepsilon_{ijk} \alpha_\ell [x_j, p_\ell] p_k \\ &= i\hbar \varepsilon_{ijk} \alpha_j p_k \end{aligned} \tag{9.25c}$$

$$\begin{aligned} [\mathbf{L}, H] &= i\hbar \boldsymbol{\alpha} \times \mathbf{p} \\ &\neq 0 \end{aligned} \tag{9.25d}$$

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

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

$$[\mathbf{J}, H] = 0\,, \tag{9.26a}$$

i.e.

$$[\mathbf{S}, H] = -i\hbar \boldsymbol{\alpha} \times \mathbf{p} \tag{9.26b}$$

and of course

$$[S_i, S_j] = i\hbar \varepsilon_{ijk} S_k \tag{9.26c}$$

claim:

$$\begin{aligned} \mathbf{S} &= \frac{\hbar}{2} \sum \\ &= \frac{-i\hbar}{2} \alpha^1 \alpha^2 \alpha^3 \boldsymbol{\alpha} \\ &= \frac{\hbar}{2} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \end{aligned} \tag{9.26d}$$

Proof:

$$[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k \tag{9.27a}$$

$$\begin{aligned}[S_i, H] &= \frac{-i\hbar}{2}\left[\alpha^1\alpha^2\alpha^3\alpha^i, H\right] \\ &= \frac{-i\hbar}{2}\frac{1}{2}\left[\alpha^j\alpha^k, \alpha^n p^n + \beta mc^2\right]\end{aligned} \tag{9.27b}$$

with

$$\left[\alpha^j\alpha^k, \beta\right] = 0 \tag{9.27c}$$

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

$$\left[P^i, P^j\right] = 0 \tag{9.28a}$$

$$\left[J^i, J^j\right] = i\hbar\varepsilon^{ijk}J^k \tag{9.28b}$$

$$\left[J^i, P^j\right] = i\hbar\varepsilon^{ijk}P^k \tag{9.28c}$$

coordinate transformation:

$$\begin{aligned}\mathbf{x} &\to \mathbf{x}' \\ &= R\mathbf{x} + \mathbf{a}\end{aligned} \tag{9.28d}$$

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

$$\begin{aligned}|\psi\rangle &\to |\psi'\rangle \\ &= U(R, a)\,|\psi\rangle\end{aligned} \tag{9.28e}$$

in relativity add boosts

$$x^\mu \to \Lambda^\mu{}_\nu x^\nu + a^\mu \tag{9.28f}$$

$$[K_i, K_j] = -i\hbar\varepsilon_{ijk}J_k \tag{9.28g}$$

$$[K_i, J_i] = i\hbar\varepsilon_{ijk}K_k \tag{9.28h}$$

generator

$$J^{\mu\nu} = \begin{cases} J_{0i} = -J_{i0} = K_i \\ J_{ij} = -J_{ji} = i\varepsilon_{ijk}J_k \end{cases} \tag{9.28i}$$

6 generators $+4$ P^μ

9.4.2 Lie algebra of generators

$$[P_\mu, P_\nu] = 0 \tag{9.29a}$$

$$[J_{\mu\nu}, J_{\rho\sigma}] = i\hbar\left(g_{\nu\rho}J_{\mu\sigma} - g_{\mu\rho}J_{\nu\sigma} - g_{\nu\sigma}J_{\mu\rho} + g_{\mu\sigma}J_{\nu\rho}\right) \tag{9.29b}$$

$$[P_\mu, J_{\rho\sigma}] = i\hbar\left(g_{\mu\rho}P_\sigma - G_{\mu\sigma}P_\rho\right) \tag{9.29c}$$

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

$$\begin{aligned} |p\rangle &\to |\Lambda p\rangle \\ &= U(\Lambda)\,|p\rangle \end{aligned} \tag{9.29d}$$

$P_\mu P^\mu$ 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

$$p^\mu = L^\mu{}_\nu q^\nu \tag{9.30a}$$

i.e. for any q^μ with

$$\begin{aligned} q^2 &= m^2 \\ &> 0 \end{aligned} \tag{9.30b}$$

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

$$p = L(p)q \tag{9.30c}$$

is in rest frame … under any LT, Λ

$$\begin{aligned} |p\rangle &\to U(\Lambda)\,|p\rangle \\ &= U(\Lambda)U\left(L(p)\right)|q\rangle \end{aligned} \tag{9.30d}$$

$$U\left(L\left(\Lambda p\right)\right)U^{-1}\left(L\left(\Lambda p\right)\right)U(\Lambda)U\left(L(p)\right)|q\rangle \tag{9.30e}$$

$$U\left(L\left(\Lambda p\right)\right)\cdot U\left(L^{-1}\left(\Lambda p\right)\right)U(\Lambda)U\left(L\left(p\right)\right)|q\rangle \tag{9.30f}$$

$$U\left(L\left(\Lambda p\right)\right)U\left(L^{-1}\left(\Lambda p\right)\Lambda\cdot L\left(p\right)\right)|q\rangle \tag{9.30g}$$

$\rightarrow$ additional labels in $|p, s\rangle$ are affected by rotations only

$$\begin{aligned} |p, s\rangle &\rightarrow U(\Lambda)\,|p, s\rangle \\ &= U\left(L\left(\Lambda p\right)\right) \underbrace{\sum D_{ss'}}_{\text{def. transformation under rotations}} \\ &= \sum D_{ss'}\,|\Lambda p, s'\rangle \end{aligned} \tag{9.31a}$$

9.4.3 2nd casimir operator

$$W_\mu W^\mu = -m^2\hbar^2 s\left(s+1\right) \tag{9.32a}$$

Pauli-Lubanski (axial) vector

$$W_\mu = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma} J^{\nu\rho} P^\sigma \tag{9.32b}$$

in rest frame

$$P^\sigma = (m, 0, 0, 0) \tag{9.32c}$$

$$W_\mu = (0, \boldsymbol{\omega}) \tag{9.32d}$$

$$\begin{aligned} W_i &= -\frac{1}{2}\varepsilon_{i\nu\rho\sigma} J^{\nu\rho} P^\sigma \\ &= -\frac{m}{2}\varepsilon_{i\nu\rho\sigma} J^{\nu\rho} \\ &= -mJ_i \end{aligned} \tag{9.32e}$$

9.5 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:

$$p^\nu \rightarrow p^\nu + \frac{e}{c}A^\nu \tag{9.33a}$$

write

$$\psi = \begin{pmatrix} \chi \\ \eta \end{pmatrix}, \quad \text{2-componenent-spinors} \tag{9.33b}$$

$$\not{p} + \frac{e}{c}\not{A} - mc \tag{9.33c}$$

$$\begin{aligned} \begin{pmatrix} \chi \\ \eta \end{pmatrix} &= \begin{pmatrix} \frac{E}{c} + \frac{e}{c}\phi - mc & -\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma} \\ \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma} & -\left(\frac{E}{c} + \frac{e}{c}\phi + mc\right) \end{pmatrix} \begin{pmatrix} \chi \\ \eta \end{pmatrix} \\ &= 0 \end{aligned} \tag{9.33d}$$

$$\Rightarrow \left(\frac{E}{c} + \frac{e}{c}\phi - mc\right)\chi = \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma}\eta \tag{9.33e}$$

$$\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma}\chi = \left(\frac{E}{c} + mc + \frac{e}{c}\phi\right)\eta \tag{9.33f}$$

$$\begin{aligned} \rightsquigarrow \eta &= \frac{\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma}}{\frac{E}{c} + mc + \frac{e}{c}\phi}\chi \\ &\approx \frac{\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \sigma}{2mc}\chi \end{aligned} \tag{9.33g}$$

Putting Eq. 9.33g in Eq. 9.33e gives us

$$\begin{aligned} \left(\frac{E}{c} + \frac{e}{c}\phi - mc\right)\chi &= \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma} \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \cdot \boldsymbol{\sigma}\frac{1}{2mc}\chi \\ &= \frac{1}{2mc}\Bigg(\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 \\ &\quad + i\left(-i\hbar\right)\frac{e}{c}\underbrace{\left(\boldsymbol{\nabla} \times \mathbf{A} + \mathbf{A} \times \boldsymbol{\nabla}\right)}_{[\nabla \times \mathbf{A}]} \cdot \boldsymbol{\sigma}\Bigg)\chi \end{aligned} \tag{9.33h}$$

"derivative within [·] only"

$$\begin{aligned} &\Rightarrow \left(\frac{1}{2m}\left(\mathbf{p} \cdot \frac{e}{c}\mathbf{A}\right)^2 + \frac{\hbar e}{2mc}\boldsymbol{\sigma} \cdot \mathbf{B} - e\phi\right)\chi \\ &= \left(E - mc^2\right)\chi \\ &=: E'\chi \end{aligned} \tag{9.33i}$$

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

$$\begin{aligned} H &\sim \boldsymbol{\mu}\cdot\mathbf{B} \\ &= \frac{e}{2m}g\mathbf{S}\cdot\mathbf{B} \\ &= \frac{e}{4m}g\boldsymbol{\sigma}\cdot\mathbf{B} \end{aligned} \tag{9.33j}$$

$$\Rightarrow g = 2 \tag{9.33k}$$

Let's do this more systematically (expand in $\frac{|e|}{m}$)
Find transformation

$$\psi = e^{-iS}\psi', \quad \text{(Foldy-Wontthuysen transformation)} \tag{9.34a}$$

such thath odd operators are suppressed by $\left(\frac{|p|}{m}\right)^n \rightsquigarrow$ mixes χ and η

$$\sigma := c\boldsymbol{\alpha}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right) \tag{9.34b}$$

$$\begin{aligned} i\hbar\partial_t\psi' &= i\hbar\partial_t e^{iS}\psi \\ &= i\hbar\left[\partial_t e^{iS}\right]\psi + e^{@S}i\hbar\partial_t\psi \\ &= i\hbar\left[\partial_t e^{+iS}\right]e^{-iS}\psi' + e^{iS}He^{-iS}\psi' \\ &=: H'\psi' \end{aligned} \tag{9.34c}$$

$$\begin{aligned} H' = H &+ i\left[S, H\right] + \frac{i^2}{2!}\left[S,\left[S,H\right]\right] + \frac{i^3}{3!}\dots \\ &- \hbar\dot{S} - \frac{i\hbar}{2!}\left[S,\dot{S}\right] - \frac{i^2\hbar}{3!}\left[S,\left[S,\dot{S}\right]\right]\dots \end{aligned} \tag{9.34d}$$

Recall

$$H = \beta mc^2 + \sigma + \xi, \quad \text{even: } \xi = -e\phi \tag{9.34e}$$

Set

$$S = \frac{-i\beta}{2mc^2}\sigma \tag{9.34f}$$

Compute

$$\begin{aligned} i\left[S,H\right] &= i\left[\frac{-i\beta}{2mc^2}\sigma, \beta mc^2 + \sigma + \xi\right] \\ &= \frac{\beta}{2mc^2}\left[\sigma,\xi\right] + \frac{\beta}{mc^2}\sigma^2 - \sigma \end{aligned} \tag{9.34g}$$

$$[\beta\sigma, \sigma] = \beta\sigma\sigma - \sigma\beta\sigma \\ = 2\beta\sigma^2 \tag{9.35a}$$

$$[\beta\sigma, \beta] = c\,[\beta\boldsymbol{\alpha}, \beta]\left(+ \frac{e}{c}\mathbf{A}\right) \\ = -2\sigma \tag{9.35b}$$

$$H' = \beta mc^2 + \frac{\sigma^2}{2mc^2} - \frac{\sigma^4}{8m^3c^6} + \varepsilon - \frac{[\sigma,[\sigma,\varepsilon]]}{8m^2c^4} - \frac{i\hbar\,[\sigma,\sigma]}{8m^2c^4} \leftarrow (\text{even}) \\ + \frac{\beta}{2mc^2}\,[\sigma,\varepsilon] - \frac{\sigma^3}{2m^2c^4} + \frac{i\hbar\beta\sigma}{2mc^2} (\leftarrow \text{add, suppressed by at least } \frac{1}{m}) \tag{9.36a}$$

repeat

$$\psi' = e^{iS'}\psi'' \tag{9.36b}$$

with

$$S' = \frac{-i\beta\sigma'}{2mc^2} \tag{9.36c}$$

$$H'' = H_{\text{even}} + \sigma'' \tag{9.36d}$$

suppressen by $\frac{1}{m^2}$ 3rd and last iteration

$$H''' =: H \\ = \beta c^2 + \frac{\sigma^2}{2mc^2} - \frac{\sigma^4}{8m^3c^6} + \varepsilon - \frac{[\sigma,[\sigma,\varepsilon]]}{8m^2c^4} - \frac{i\hbar\,[\sigma,\sigma]}{8m^2c^4} + \mathcal{O}\left(\frac{1}{m^3}\right) \tag{9.36e}$$

$$\frac{\sigma^2}{2mc^2} = \frac{1}{2m}\alpha_i\left(p_i + \frac{e}{c}A_i\right)\alpha_j\left(p_j + \frac{e}{c}A_j\right) \\ = \frac{1}{2m}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 + \frac{\hbar e}{2m}\boldsymbol{œ}\cdot\boldsymbol{\beta} \tag{9.37a}$$

$$\frac{-\sigma^4}{8m^3c^6} = \frac{\mathbf{p}^4}{8m^3c^2} + \ldots \text{relativistic correction to kinetic energy} \tag{9.37b}$$

$$-\frac{1}{8m^2c^4}\,[\sigma,[\sigma,\varepsilon]] = \frac{(-i\hbar)^2}{8m^2c^2}\left(\alpha_i\nabla_i\,[\alpha_j\nabla_j, eV]\right) \tag{9.37c}$$

where

$$[\alpha_j\nabla_j, eV] = \alpha_j e\left(\nabla_j V - V\nabla_j\right) \\ = \alpha_i e\left(\nabla_j V\right) \tag{9.37d}$$

which gives us

$$-\frac{1}{8m^2c^4}\left[\sigma,\left[\sigma,\varepsilon\right]\right]=\frac{\left(i\hbar^2\right)}{8m^2c^2}\left[\alpha_i\nabla_i,\alpha_jE_j\right] \tag{9.37e}$$

where

$$\begin{aligned}\left[\alpha_i\nabla_i,\alpha_jE_j\right]&=\alpha_i\alpha_j\nabla_i\cdot E_i-\alpha_j\alpha_iE_j\nabla_i\\&=\nabla\cdot E+i\sigma\left(\nabla\times E\right)-E\cdot\nabla-i\sigma\left(E\times\nabla\right)\\&=\left(\nabla\cdot E\right)-2i\boldsymbol{\sigma}\left(\mathbf{E}\times\boldsymbol{\nabla}\right)+i\sigma\left[\boldsymbol{\nabla}\times\mathbf{E}\right]\end{aligned} \tag{9.37f}$$

which leads to

$$\begin{aligned}\frac{-\sigma^4}{8m^3c^6}&=\frac{ie\hbar^2}{4m^2c^2}\left(\underbrace{\boldsymbol{\sigma}\cdot\left(\mathbf{E}\times\boldsymbol{\nabla}\right)}_{\text{spin orbit}}-\underbrace{\frac{\sigma\left(\boldsymbol{\nabla}\times\mathbf{E}\right)}{2}}_{\text{=0 Coulomb}}-\underbrace{\frac{\hbar^2e}{8m^2c^2}\left(\boldsymbol{\nabla}\cdot\mathbf{E}\right)}_{\text{Darwin term}}\right)\\&=\frac{1}{2m^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\cdot\mathbf{S}\cdot\mathbf{L}\end{aligned} \tag{9.37g}$$

and

$$\frac{-\hbar}{4m^2c^2}\boldsymbol{\sigma}\left(-\frac{\mathrm{d}V}{\mathrm{d}r}\cdot\mathbf{S}\cdot\mathbf{L}\right)=\frac{1}{2m^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\cdot\mathbf{S}\cdot\mathbf{L} \tag{9.37h}$$

and

$$\frac{\hbar^2}{8m^2c^2}\left(\boldsymbol{\nabla}\left(-cE\right)=\frac{\hbar^2}{8mc^2}\nabla\left(\nabla V\right)\right)=\frac{+i\hbar^2Ze^3}{2m^2c^2\delta(r)} \tag{9.37i}$$

where we have used

$$\Delta\left(\frac{1}{r}\right)=-4\pi\delta(\mathbf{r}) \tag{9.37j}$$

and $Z=1$

including all other terms

- $-i\hbar\boldsymbol{\nabla}\rightarrow-i\hbar\boldsymbol{\nabla}+\frac{e}{c}\mathbf{A}$ (gauge symmetry)
- $\mathbf{E}=-\boldsymbol{\nabla}\phi-\frac{1}{c}\dot{\mathbf{A}}$ (internal symmetry)

Chapter 10

Second Quantization

Classical field theory $\rightarrow$ quatized field theory "done" already for radiation field, section 5 $\rightarrow$ 8

10.1 Creation and annihilation operators for bosons and fermions

Bosons: recall radiation field $\hat{a}_{\mathbf{k}\lambda}$, $\hat{a}^{\dagger}_{\mathbf{k}\lambda}$ ($\hat{\cdot}$: bosons, Signer will forget $\hat{\cdot}$ ...) now $i \sim \{\mathbf{k}, \lambda\}$. Discrete

$$[\hat{a}_i, \hat{a}_j] = \left[\hat{a}^{\dagger}_i, \hat{a}^{\dagger}_j\right] \tag{10.1a}$$
$$= 0$$
$$\left[\hat{a}_i, \hat{a}^{\dagger}_j\right] = \delta_{ij}, \quad \text{(discrete)} \tag{10.1b}$$

states

$$|n_1, n_2, \ldots, n_m\rangle = \frac{\left(\hat{a}^{\dagger}_1\right)^{n_1} \ldots \left(\hat{a}^{\dagger}_m\right)^{n_m}}{\sqrt{n_1! \ldots n_m!}} |0\rangle \tag{10.1c}$$
$$\hat{a}_i |0\rangle = 0 \tag{10.1d}$$

fermions: the same exept

$$[\cdot, \cdot] \equiv [\cdot, \cdot]_- \tag{10.2a}$$
$$\rightarrow \{\cdot, \cdot\} \equiv [\cdot, \cdot]_+ \tag{10.2b}$$

$$\left\{\hat{b}_i, \hat{b}^{\dagger}_j\right\} = \delta_{ij} \tag{10.3a}$$
$$\left\{\hat{b}_i, \hat{b}_j\right\} = \left\{\hat{b}^{\dagger}_i, \hat{b}^{\dagger}_j\right\} \tag{10.3b}$$
$$= 0$$
$$\left(\hat{b}^{\dagger}_i\right)^2 = 0 \tag{10.3c}$$
$$n_i = \{0, 1\}, \quad \text{Pauli} \tag{10.3d}$$

particularly:

$$|1\rangle = \hat{b}_i^\dagger |0\rangle \tag{10.3e}$$

$$\begin{aligned}\hat{b}_i^\dagger |1\rangle &= \left(\hat{b}_i^\dagger\right)^{\pm} |0\rangle \\ &= 0\end{aligned} \tag{10.3f}$$

$$\begin{aligned}|n_1 = 1, n_2 = 1\rangle &= \hat{b}_1^\dagger \hat{b}_2^\dagger |0\rangle \\ &= -\hat{b}_2^\dagger b_1^\dagger |0\rangle \\ &= -|n_2 = 1, n_1 = 1\rangle\,, \quad \text{antisymmetric}\end{aligned} \tag{10.3g}$$

$$\langle n_1 \dots n_m | n_1' \dots n_m'\rangle = \delta_{n1,n_1'} \dots \delta_{n_m n_m'}, \quad \text{orthogonality} \tag{10.3h}$$

$$\sum_{n_i} |n_1 \dots n_m\rangle\langle n_1 \dots n_m| = \mathbf{1}, \quad \text{completeness} \tag{10.3i}$$

$$\begin{aligned}n &= \sum_i n_i \\ &= \sum_i \hat{b}_i^\dagger \hat{b}_i, \quad \text{counting operator}\end{aligned} \tag{10.3j}$$

10.2 Field operators

Let $\psi_i(x)$ wave function (coord. rep. of state) x : here 3-vector not 4-vector any more

$$\to \text{basis} \int \mathrm{d}^3x\, \psi_i^*(x)\psi_j(x) = \delta_{ij} \tag{10.4a}$$

(can think of ψ_i as eigenfunctions of H, $H\psi_i = E\psi_i$)
consider any state $\to f(x) \in L^2$

$$\begin{aligned}f(x) &= \sum_i c_i \psi_i(x) \\ &= \int \mathrm{d}^3\mathbf{y}\, f(y) \underbrace{\sum_i \psi_i^*(y)\psi_i(x)}_{\delta^{(3)}(\mathbf{x}-\mathbf{y})}\end{aligned} \tag{10.4b}$$

with

$$c_i = \int \mathrm{d}^3\mathbf{y}\, \psi_i^*(y) f(y) \tag{10.4c}$$

$$\hat{\psi}(\mathbf{x}) = \sum \hat{a}_i \psi_i(\mathbf{x}) \tag{10.5a}$$

$$\hat{\psi}^\dagger = \sum \hat{a}_i^\dagger \psi_i^*(x) \tag{10.5b}$$

$$\begin{aligned}\hat{\psi}^\dagger \left|0\right\rangle &= \sum_j |j\rangle\langle j| \sum_i \hat{a}_i^\dagger \psi_i^* \left|0\right\rangle \\ &= \sum_{j,i} |j\rangle \left\langle 0\right| \hat{a}_j \hat{a}_i^\dagger \left|0\right\rangle \psi_i^\dagger(x)\,,\end{aligned} \tag{10.5c}$$

where

$$\begin{aligned}\hat{a}_j \hat{a}_i^\dagger &= \left[\hat{a}_j, \hat{a}_i^\dagger\right]_\mp \pm \hat{a}_i^\dagger \hat{a}_j \\ &= \delta_{ij} \pm \text{does not contribute}\end{aligned} \tag{10.5d}$$

$$\begin{aligned}\rightsquigarrow \hat{\psi}^\dagger(x) &= \sum_i |i\rangle\, \psi_i^*(x) \\ &= \sum |i\rangle \left\langle i\right| x\rangle \\ &= |x\rangle\end{aligned} \tag{10.5e}$$

$\hat{\psi}^\dagger(\mathbf{x})$ creates a particle localized at $\mathbf{x}$
$\hat{\psi}(\mathbf{x})$ annihilates a particle localized at $\mathbf{x}$

$$\begin{aligned}\left[\hat{\psi}(x), \hat{\psi}(y)\right]_\mp &= \left[\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(y)\right] \\ &= 0\end{aligned} \tag{10.6a}$$

$$\begin{aligned}\left[\hat{\psi}(x), \hat{\psi}(y)\right]_\mp &= \sum_j \psi_i(x)\psi_j^*(y) \underbrace{\left[\hat{a}_i, \hat{a}_j^\dagger\right]_\mp}_{\delta_{ij}} \\ &= \sum_i \psi_i(x)\psi_j^*(g) \\ &= \delta\left(\mathbf{x} - \mathbf{y}\right)\end{aligned} \tag{10.6b}$$

Many particle states

$$|\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\rangle = \frac{1}{\sqrt{n!}}\hat{\psi}^\dagger(\mathbf{x}_1)\ldots\hat{\psi}(\mathbf{x}_n)\,|0\rangle \tag{10.7}$$

Example: Two identical bosons/fermions at $\mathbf{x}_1 \& \mathbf{x}_2$:

$$\begin{aligned}\psi_{ij}\left(\mathbf{x}_1, \mathbf{x}_2\right) &= \langle \mathbf{x}_1, \mathbf{x}_2 | \, ij\rangle \\ &= \frac{1}{\sqrt{2}}\,\langle 0|\,\hat{\psi}(\mathbf{x}_2)\hat{\psi}(x_1)\hat{a}_i^\dagger\hat{a}_j^\dagger\,|0\rangle \\ &= \frac{1}{\sqrt{2}}\sum_{n,m}\langle 0|\,\hat{a}_m\hat{a}_n\hat{a}_i^\dagger\hat{a}_j^\dagger\,|0\rangle\,\psi_m(\mathbf{x}_2)\psi_1(\mathbf{x}_1)\end{aligned} \tag{10.8a}$$

where

$$\langle 0|\,\hat{a}_m\hat{a}_n\hat{a}_i^\dagger\hat{a}_j^\dagger\,|0\rangle = \delta_{n_1 m_j} \pm \delta_{m_i}\delta_{n_j}\begin{cases} + & \text{bosons} \\ - & \text{fermions}\end{cases} \tag{10.8b}$$

$$\begin{aligned}&\rightsquigarrow \psi_{ij}\left(\mathbf{x}_1, \mathbf{x}_2\right) \\ &\quad = \frac{1}{\sqrt{2}}\left(\psi_j(\mathbf{x}_2)\psi_1(\mathbf{x}_1) \pm \psi_i(\mathbf{x}_2)\psi_j(\mathbf{x}_1)\right), \\ &\qquad \text{(bosons symmetric, fermions antisummetric (Slater determinant))}\end{aligned} \tag{10.8c}$$

For fixed number n of particles Hilbert space $\mathcal{H}_n$

$$\hat{\psi}^\dagger(\mathbf{x})\mathcal{H}_n \to \mathcal{H}_{n-1} \tag{10.8d}$$

$$\hat{\psi}(\mathbf{x})\mathcal{H}_n \to \mathcal{H}_{n-1} \tag{10.8e}$$

Fock space

$$\begin{aligned}\mathcal{F} &= \bigoplus_{n=0}^{\infty}\mathcal{H}_n \\ &= \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \ldots\end{aligned} \tag{10.8f}$$

with $\mathcal{H}_0$ Volume $|0\rangle$

10.3 Observables in 2nd quantization

Observables expressed in terms of fields $/to$ operators in Fock space $\mathcal{F}$.
Example: particle number density

QM: probability density

$$\rho(x) = |\psi(x)|^2 \tag{10.9}$$

now:

$$\begin{aligned}
\hat{\rho(x)} &= \hat{\psi}^\dagger(x)\hat{\psi}(x) \\
&= \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \psi_i^*(x)\psi_j(x) \\
&= \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \langle x|\, i\rangle \langle j|\, x\rangle
\end{aligned} \tag{10.10a}$$

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{x}\, \hat{\rho}(x) &= \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \langle j| \underbrace{\int \mathrm{d}^3 x\, |x\rangle\langle x|}_{\mathbf{1}} |i\rangle \\
&= \sum_i \hat{a}_i^\dagger \hat{a}_i \\
&= \sum_i n_i
\end{aligned} \tag{10.10b}$$

$$\hat{T} = \int \mathrm{d}^3\mathbf{x}\, \hat{\psi}^\dagger \left(-\frac{\hbar^2\nabla^2}{2m}\right) \hat{\psi}(x) \tag{10.11a}$$

$$\hat{\psi}(x) = \sum_i \hat{a}_i \psi_i(x) \tag{10.12a}$$

$$\hat{\psi}^\dagger(x) = \sum_i \hat{a}_i^\dagger \tag{10.12b}$$

$$\hat{\psi}(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \hat{a}_k e^{-i\mathbf{k}\cdot\mathbf{x}} \tag{10.12c}$$

$$\hat{\psi}^\dagger(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \hat{a}_k^\dagger e^{i\mathbf{k}\cdot\mathbf{x}} \tag{10.12d}$$

$$\begin{aligned}\hat{T} &= \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3 k'}{(2\pi)^3} \underbrace{e^{i\mathbf{x}\left(\mathbf{k}-\mathbf{k}'\right)}}_{(2\pi)^3\delta\left(\mathbf{k}-\mathbf{k}'\right)} \hat{a}_k^\dagger \hat{a}_{k'} \left(-\frac{\hbar^2\left(i\mathbf{k}'\right)^2}{2m}\right) \\ &= \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\hbar^2\mathbf{k}^2}{2m} \underbrace{\hat{a}_k^\dagger \hat{a}_k}_{N_k}\end{aligned} \tag{10.12e}$$

N_k counts number of particles of kind k. Potential

$$U(x) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{-i\mathbf{q}\cdot\mathbf{x}} \tilde{U}(\mathbf{q}) \tag{10.12f}$$

$$\begin{aligned}\hat{U} &= \int \mathrm{d}^3\mathbf{x}\, \hat{\psi}^\dagger(x) U(x) \hat{\psi}(x) \\ &= \int \frac{\mathrm{d}^3 k_1}{(2\pi)^3} \int \frac{\mathrm{d}^3 \mathbf{k}_2}{(2\pi)^3} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \int \underbrace{\mathrm{d}^3 x\, e^{i\mathbf{k}_1\cdot\mathbf{x}} e^{-i\mathbf{k}_2\cdot\mathbf{x}} e^{-i\mathbf{q}\cdot\mathbf{x}}}_{(2\pi)^3\delta(\mathbf{k}_1-\mathbf{k}_2-\mathbf{q})} \hat{a}_{k_1}^\dagger \hat{a}_{k_2} \tilde{U}(\mathbf{q}) \\ &= \int \frac{\mathrm{d}^3 \mathbf{k}_1}{(2\pi)^3} \int \frac{\mathrm{d}^3 \mathbf{k}_2}{(2\pi)^3} \tilde{U}(\mathbf{k}_1\mathbf{k}_2)\end{aligned} \tag{10.12g}$$

$$\begin{aligned}V(x_1, x_2) &= V(x_1 - x_2) \\ &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{-i\mathbf{q}(\mathbf{x}_1-\mathbf{x}_2)} \tilde{V}(q)\end{aligned} \tag{10.12h}$$

$$\begin{aligned}\hat{V} &= \int \mathrm{d}^3x_1 \int \mathrm{d}^3x_2 \, \hat{\psi}^\dagger(x_1)\,\hat{\psi}^\dagger(x_2) V(x_1 - x_2)\,\hat{\psi}(x_1)\hat{\psi}(x_2) \\ &= \int \prod_{i=1}^{4} \frac{\mathrm{d}k_i}{(2\pi)^3} \int \frac{\mathrm{d}^3q}{(2\pi)^3} \cdot \int \mathrm{d}^3x_1 \, e^{i\mathbf{x}_1(\mathbf{k}_1-\mathbf{k}_3-\mathbf{q})} \\ &\quad \cdot \int \mathrm{d}^3x_2 \, e^{i\mathbf{x}_2(\mathbf{k}_2-\mathbf{k}_4+\mathbf{q})} \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\hat{a}_{k_3}\hat{a}_{k_4} \\ &= \int \frac{\mathrm{d}^3\mathbf{k}_1}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}_2}{(2\pi)^3} \int \frac{\mathrm{d}^3q}{(2\pi)^3} \, \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\hat{a}_{\mathbf{k}_1-\mathbf{q}}\hat{a}_{\mathbf{k}_2+\mathbf{q}}\tilde{V}(q)\end{aligned} \tag{10.12i}$$

consider commutation relation between field operators:

$$\left[\hat{\psi}(x), \hat{\psi}(y)\right]_{\mp} = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3} \, e^{-i\mathbf{k}\cdot\mathbf{x}} e^{+i\mathbf{k}'\cdot\mathbf{y}} \underbrace{\left[\hat{a}_k, \hat{a}^\dagger_{k'}\right]}_{(2\pi)^3\delta\left(\mathbf{k}-\mathbf{k}'\right)} \stackrel{!}{=} \delta(\mathbf{x} - \mathbf{y}) \tag{10.13a}$$

with the $(2\pi)^3$ of $(2\pi)^3\,\delta\left(\mathbf{k} - \mathbf{k}'\right)$ being convection and generalization of

$$\left[\hat{a}_i, \hat{a}^\dagger_j\right] = \delta_{ij} \tag{10.13b}$$

time dependence of field operator: Schrödinger picture $\rightarrow$ Heisenberg

$$\underbrace{\hat{\psi}(\mathbf{x}, t)}_{\text{Heisenberg}} = e^{\frac{i}{\hbar}\hat{H}t} \underbrace{\hat{\psi}(\mathbf{x})}_{\text{SChrödinger}} e^{\frac{-i}{\hbar}\hat{H}t} \tag{10.14a}$$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{x}, t) &= -\left[\hat{H}, \hat{\psi}(\mathbf{x}, t)\right] \\ &= -\left[\hat{H}, \hat{\psi}(\mathbf{x})\right] \\ &= -e^{\frac{i}{\hbar}\hat{H}t}\left[\hat{H}, \hat{\psi}(x)\right] e^{-\frac{i}{\hbar}\hat{H}t}\end{aligned} \tag{10.14b}$$

take free case

$$\hat{H} = \hat{T}, \quad \text{bosons} \tag{10.14c}$$

$$\left[\hat{T}, \hat{\psi}(x)\right] = \int \mathrm{d}^3y \, \frac{\hbar^2}{2m} \left[\nabla_y \psi^\dagger(y) \nabla_y \hat{\psi}(y), \hat{\psi}(x)\right] \tag{10.14d}$$

from now on, don't write ∇_y but ∇

$$\begin{aligned}
\left[\nabla_y \psi^\dagger(y) \nabla_y \hat{\psi}(y), \hat{\psi}(x)\right] &= \nabla \hat{\psi}^\dagger(y) \varsigma \hat{\psi}(y) \hat{\psi}(x) - \hat{\psi}(x) \nabla \hat{\psi}^\dagger(y) \nabla \hat{\psi}(y) \\
&= \nabla \hat{\psi}^\dagger(y) \hat{\psi}(x) \nabla \hat{\psi}(y) - \hat{\psi}(x) \nabla \hat{\psi}^\dagger(y) \nabla \hat{\psi}(y) \\
&= \nabla \Big(\left[\hat{\psi}^\dagger(y), \hat{\psi}(x)\right] \\
&\quad + \hat{\psi}(x) \underbrace{\hat{\psi}^\dagger(y) \Big) \nabla \hat{\psi}(y) - \hat{\psi}(x) \nabla \hat{\psi}^\dagger(y) \nabla \hat{\psi}(y)}_{=0} \\
&= \int \mathrm{d}^3 y \, \frac{-\hbar^2}{2m} \nabla_y \delta\left(\mathbf{x} - \mathbf{y}\right) \nabla \hat{\psi}(y) \\
&= \frac{\hbar^2}{2m} \nabla_x^2 \hat{\psi}(x)
\end{aligned}$$

in free case

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(x,t) = -\frac{\hbar^2}{2m} \nabla^2 \hat{\psi}\left(x,t\right) + \diamondsuit \tag{10.14e}$$

$\diamondsuit$ with interations much more complicated $\rightarrow$ QFT

10.4 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 $\Phi(\mathbf{x}, t) = \Phi(x)$

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$$\mathcal{L} = \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} \underbrace{\frac{m^2 c^2}{\hbar^2}}_{\equiv m^2} \Phi^2 - \underbrace{V(\Phi)}_{=0} \tag{10.15a}$$

free field (no interactions). Action:

$$\begin{aligned} S &= \int \mathrm{d}t \int \mathrm{d}^3x\, \mathcal{L} \\ &= \int \mathrm{d}^3 4x\, \mathcal{L}\left(\Phi, \partial_\mu \Phi\right) \end{aligned} \tag{10.15b}$$

$$\delta S = 0 \tag{10.15c}$$

$$\rightarrow \frac{\partial \mathcal{L}}{\partial \Phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \Phi\right)} 90 \tag{10.15d}$$

for our $\mathcal{L}$:

$$-m^2\Phi - \partial_\mu \partial^\mu \Phi = 0 \tag{10.15e}$$

Klein-Gordan equation

- Conjugate momentum field

$$\begin{aligned} \pi\left(\mathbf{x}, t\right) &= \frac{\partial \mathcal{L}}{\partial \Phi} \\ &= \dot{\phi}\left(\mathbf{x}, t\right) \end{aligned} \tag{10.16a}$$

Hamiltonian

$$\begin{aligned} H &= \int \mathrm{d}^3\mathbf{x}\, \pi \dot{\Phi} - L \\ &= \int \mathrm{d}^3x\, \left(\pi\dot{\phi} - \mathcal{L}\right) \\ &= \frac{1}{2}\int \mathrm{d}^3x\, \left(\pi^2 + \left(\nabla\Phi\right)^2 + m^2\Phi^2\right) \end{aligned} \tag{10.16b}$$

with $\mathcal{L}$ the Lagrangian density

$$\begin{aligned} \int \mathrm{d}^3x\, \mathcal{L} &= L \\ &= \text{Lagriangian} \end{aligned} \tag{10.16c}$$

- now second quantization:

$$\Phi(x) \rightarrow \Phi\hat{(x)} \tag{10.17a}$$

and

$$\pi(x) \to \hat{\pi}(x) \tag{10.17b}$$

$$\begin{aligned}\left[\hat{\phi}\left(\mathbf{x},t\right),\hat{\phi}\left(\mathbf{y},t\right)\right] &= \left[\hat{\pi}\left(\mathbf{x},t\right),\hat{\pi}\left(\mathbf{y},t\right)\right] \\ &= 0\end{aligned} \tag{10.17c}$$

impose

$$\left[\hat{\Phi}\left(\mathbf{x},t\right),\hat{\pi}\left(\mathbf{y},t\right)\right] = i\delta\left(\mathbf{x}-\mathbf{y}\right) \tag{10.17d}$$

$$\sim [x_i, p_j] = i\delta_{ij}, \quad (\hbar = 1) \tag{10.17e}$$

spin 0, bosonic field use $[\cdot,\cdot] = [\cdot,\cdot]_-$ and not $\{\cdot,\cdot\} = [\cdot,\cdot]_+$

now as for radiation field

$$\hat{\Phi}\left(\mathbf{x},t\right) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{2\omega_k}\left(\hat{a}_k e^{i\mathbf{kx}-i\omega_k t} + \hat{a}_k^\dagger e^{-i\mathbf{kx}+i\omega_k t}\right) \tag{10.17f}$$

with $\omega_k = \sqrt{\mathbf{k}^2 + m^2}$ this satisfies KGE

$$\begin{aligned}\hat{\pi}\left(\mathbf{x},t\right) &= \dot{\hat{\Phi}}\left(\mathbf{x},t\right) \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{2\omega_k}\left(-i\omega_k\hat{a}_k e^{i\mathbf{kx}-i\omega_k t} + i\omega_k\hat{a}_k^\dagger e^{-i\mathbf{kx}+i\omega_k t}\right)\end{aligned} \tag{10.17g}$$

Note: change in normalization:

$$\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \to \underbrace{\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2\omega_k}}_{\text{Lorentz invariant}} \tag{10.17h}$$

Proof:

$$\begin{aligned}&\int \frac{\mathrm{d}^3k}{(2\pi)^4} 2\pi\delta\left(k^2-m^2\right)\sigma(k_0), \\ &\qquad (\text{manifestly } L\text{-invariant}) = \int \frac{\mathrm{d}^4k}{(2\pi)^3}\delta\left(k^2-m^2\right)\vartheta\left(k_0\right) \\ &= \int \frac{\mathrm{d}^4k}{(2\pi)^3}\frac{1}{2\omega_k}\left(\delta\left(k_0-\omega_k\right)+\delta\left(k_0+\omega_k\right)\vartheta\left(k_0\right)\right) \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{\omega_k}\end{aligned} \tag{10.18a}$$

where in $\delta\left(k_0+\omega_k\right)$ ω_k does not contribute and we used

$$\delta\left(f(x)\right)=\sum_i \frac{1}{|f(x_i)|}\delta(x_i), \quad f(x_i)=0 \tag{10.18b}$$

Express $\hat{a}_k$ and $\hat{a}_k^\dagger$ in terms of $\hat{\phi}$ and $\hat{\pi}$

$$\int \mathrm{d}^3x\, e^{i\mathbf{k}\cdot\mathbf{x}}\left(\omega_k\hat{\phi}(\mathbf{x},t)+i\hat{\pi}\left(\mathbf{x},t\right)\right)=\ldots\hat{a}_k e^{-i\omega_k t} \tag{10.18c}$$

$$\Rightarrow \hat{a}_k=\int \mathrm{d}^3\mathbf{x}\, e^{ikx}\left(\omega_k\hat{\phi}+i\hat{\pi}\right) \tag{10.18d}$$

$$\hat{a}_k^\dagger=\int \mathrm{d}^3x\, e^{-i\mathbf{k}\mathbf{x}}\left(\omega_k\hat{\phi}-i\hat{\pi}\right) \tag{10.18e}$$

check consistency:

$$\left[\hat{a}_k,\hat{a}_{k'}^\dagger\right]=\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{y}\, e^{i\omega_k t-i\mathbf{k}\mathbf{x}}e^{-i\omega_{k'}t+i\mathbf{k}'\mathbf{x}}\left[\omega_k\hat{\phi}+i\hat{\pi},\omega_{k'}\hat{\phi}\pm i\hat{\pi}\right] \tag{10.18f}$$

where

$$\left[\omega_k\hat{\phi}+i\hat{\pi},\omega_k\hat{\phi}\pm i\hat{\pi}\right]=\left(\omega_k\mp\omega_{k'}\right)\delta\left(\mathbf{x}-\mathbf{y}\right) \tag{10.18g}$$

$$\begin{aligned}\rightsquigarrow \left[\hat{a}_k,\hat{a}_{k'}^\dagger\right]&=\int \mathrm{d}^3\mathbf{x}\, e^{-i\mathbf{x}\left(\mathbf{k}-\mathbf{k}'\right)}e^{i(\omega_k-\omega_{k'})t}\\&=\left(2\pi\right)^3 2\omega_k\delta\left(\mathbf{k}-\mathbf{k}'\right)\end{aligned} \tag{10.18h}$$

where

$$\int \mathrm{d}^3\mathbf{x}\, e^{-i\mathbf{x}\left(\mathbf{k}-\mathbf{k}'\right)}=\left(2\pi\right)^3\delta\left(\mathbf{k}-\mathbf{k}'\right) \tag{10.18i}$$

$$\begin{aligned}\rightsquigarrow \hat{H}&=\ldots\\&=\frac{1}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3}\frac{1}{2\omega_k}\omega_k\left(\hat{a}_k^\dagger\hat{a}_k+\underbrace{\hat{a}_k\hat{a}_k^\dagger}_{\hat{a}^\dagger\hat{a}_k+\sim\delta(0)}\right)\end{aligned} \tag{10.18j}$$

where $\delta(0)$ is infinite ground state energy but no absolute energy scale (only cae about energy differences)

nermal ordering: (anti) commute all $\hat{a}^\dagger$ to the left of $\hat{a}$

$$\hat{H}:=\int\frac{\mathrm{d}^3k}{\left(2\pi\right)^3}\frac{1}{2\omega_k}\left(\hat{a}_k^\dagger\hat{a}_k\right)\omega_k, \quad \text{subtracted } \langle 0|\,H\,|0\rangle=\infty \tag{10.19}$$

$$\mathcal{L} = \overline{\psi}(x)\left(i\partial\!\!\!/ - m\right)\psi(x), \quad (\hbar = 1, c = 1) \tag{10.20a}$$

$$\begin{aligned}
&\frac{\partial \mathcal{L}}{\partial \psi} - \partial^\mu \frac{\partial \mathcal{L}}{\partial\left(\partial^\mu \psi\right)} \\
&\quad = 0 \\
&\quad = -m\overline{\psi} - \partial^\mu\left(\overline{\psi} i \gamma_\mu\right) \\
&\quad = \underbrace{\overline{\psi}\left(i\partial\!\!\!/ + m\right)}_{\text{adjoint Dirac equation}} \\
&\quad = 0
\end{aligned} \tag{10.20b}$$

Field momentum conjugate to ψ

$$\begin{aligned}
\pi &\doteq \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \\
&= \overline{\psi} i \Gamma^0 i \psi^\dagger
\end{aligned} \tag{10.21a}$$

Hamiltonian

$$\begin{aligned}
H &= \int \mathrm{d}^3x \left(\pi\dot{\psi} - \mathcal{L}\right) \\
&= \int \mathrm{d}^3x \, i\psi^\dagger\dot{\psi}
\end{aligned} \tag{10.21b}$$

add $\hat{}$ and impose

$$\begin{aligned}
\left\{\hat{\psi}_\alpha(\mathbf{x}, t), \hat{\psi}_\beta(\mathbf{y}, t)\right\} &= \left\{\hat{\pi}_\alpha(\mathbf{x}, t), \hat{\pi}_\beta(\mathbf{y}, t)\right\} \\
&= 0
\end{aligned} \tag{10.21c}$$

$$\begin{aligned}
\left\{\hat{\psi}_\alpha(\mathbf{x}, t), \hat{\pi}_\beta(\mathbf{y}, t)\right\} &= i\Delta_{\alpha\beta}\delta(\mathbf{x} - \mathbf{y}), \\
&\quad \alpha, \beta \in \{1, \cdots, 4\} \text{ spinor indices}
\end{aligned} \tag{10.21d}$$

fermions $\Rightarrow$ use

$$\{\cdot, \cdot\} = [\cdot, \cdot]_+ \tag{10.22}$$

and not

$$[\cdot, \cdot] = [\cdot, \cdot]_- \tag{10.23}$$

field operators in momentum representaion

v=0

$$\hat{\psi}_\alpha = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{1}{2\omega_k} \sum_{r=1}^{2} \left(\hat{b}\left(\mathbf{k}, r\right) U_\alpha \left(k, r\right) e^{-ikx} + \hat{d}^\dagger \left(k, r\right) V_\alpha (k, r) e^{ikx} \right) \tag{10.24a}$$

where $\int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{1}{2\omega_k}$ is Lorentz invariant and $\sum_{r=1}^{2}$ from spin and $b^\dagger$ creates $E > 0$ electrons and $d^\dagger$ creates a $E > 0$ positron
satisfies Dirac, since

$$(k - m)\, u = 0 \tag{10.24b}$$

$$-k - m \tag{10.24c}$$

The anti commutation relations of the fields are consistent with

$$\begin{aligned} \left\{\hat{b}_{kr}, \hat{b}_{k'r'}\right\} &= \left\{\hat{d}_{kr}, \hat{d}^\dagger_{k'r'}\right\} \\ &= (2\pi)^3\, 2\omega_k \delta_{rr'} \delta\left(\mathbf{k} - \mathbf{k}'\right) \end{aligned} \tag{10.25a}$$

$$\begin{aligned} \left\{\hat{b}, \hat{b}\right\} &= \left\{\hat{b}^\dagger, \hat{d}^\dagger\right\} \\ &= \{b, d\} \\ &= \dots \\ &= 0 \end{aligned} \tag{10.25b}$$

Check:

$$\begin{aligned} &\left\{\hat{\psi}_\alpha, \hat{\psi}^\dagger_\beta\right\} \\ &= \int \frac{\mathrm{d}^3 k}{(2\pi)^3} 2\omega_k \int \frac{\mathrm{d}^3 k'}{(2\pi)^3\, 2\omega'_k} \sum_{?} \left(\left\{\hat{b}_{kr}, \hat{b}_{k'r'}\right\} U_\alpha\left(\mathbf{k}, r\right) U^\dagger_\beta\left(k', r'\right) e^{-ikx} e^{ik'y} \right. \\ &\qquad \left. + \left\{\hat{d}^\dagger_{kr}, \hat{d}_{k'r'}\right\} V_\alpha\left(k, r\right) V^\dagger_\beta\left(k', r'\right) e^{ikr} e^{-ik'y} \right) \\ &= \int \underbrace{\frac{\mathrm{d}^3 k}{(2\pi)^3\, 2\omega_k}}_{\text{section 9.4}} \frac{1}{2\omega_k} \sum_r \left(\left(U\left(k, r\right) \overline{U}\left(k, r\right) \gamma_0 \right)_{\alpha\beta} e^{-ik(x-y)} \right. \\ &\qquad \left. - \left(U\left(k, r\right) \overline{U}\left(k, r\right) \gamma_0 \right)_{\alpha\beta} e^{ik(x-y)} \right) \\ &= \int \frac{\mathrm{d}^3 k}{(2\pi)^3\, 2\omega_k} 2\omega_k \sum_r \left(\hat{b}^\dagger_{kr} \hat{b}_{kr} - \hat{d}_{kr} \hat{d}^\dagger_{kr} \right) \end{aligned} \tag{10.26a}$$

where

$$\left(U\left(k,r\right)\overline{U}(k,r)\gamma_0\right)_{\alpha\beta} = \left(\left(k+m\right)\gamma_0\right)_{\alpha\beta} \tag{10.26b}$$

and

$$\left(U\left(k,r\right)\overline{U}\left(k,r\right)\gamma_0\right)_{\alpha\beta} = \left(\left(-k+m\right)\gamma_0\right)_{\alpha\beta} \tag{10.26c}$$

in 2nd term change integration variable $\mathbf{k} \to -\mathbf{k}$

$$\begin{aligned}
\rightsquigarrow \left\{\hat{\psi}_\alpha, \hat{\psi}^\dagger_\beta\right\} &= \int \frac{\mathrm{d}^3\mathbf{k}}{\left(2\pi\right)^3\left(2\omega_k\right)} \left(\left(k_0\gamma_0 - \mathbf{k}\boldsymbol{\gamma} + m\right)\gamma_0\right. \\
&\qquad \left. + \left(k_0\gamma_0 + \mathbf{k}'\boldsymbol{\gamma} - m\right)\gamma_0\right)_{\alpha\beta} e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} \\
&= \int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3 2\omega_k} 2\omega_k \delta_{\alpha\beta} e^{ik(\mathbf{x}-\mathbf{y})} \\
&= \delta_{\alpha\beta}\delta\left(\mathbf{x}-\mathbf{y}\right)
\end{aligned} \tag{10.26d}$$

$$\begin{aligned}
\hat{H} &= \dots \\
&= \int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3 2\omega_k}\omega_k \sum_r \left(\hat{b}^\dagger_{kr}\hat{b}_{kr} - \hat{d}_{kr}\hat{d}^\dagger_{kr}\right)
\end{aligned} \tag{10.26e}$$

$$\hat{H} = \int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3 2\omega_k}\omega_k \sum_r \left(\hat{b}^\dagger_{kr}\hat{b}_{kr} + \hat{d}^\dagger_{kr}\hat{d}_{kr}\right) \tag{10.26f}$$

$$\begin{aligned}
\hat{Q} &= \hat{j}^0 \\
&= \overline{\hat{\psi}}\gamma^0\hat{\psi} \\
&= \dots \\
&= \int \frac{\mathrm{d}^3k}{\left(2\pi\right)^3 2\omega_k} \sum_r \left(\hat{b}^\dagger_{kr}\hat{b}_{kr} - \hat{d}^\dagger_{kr}\hat{d}_{kr}\right)
\end{aligned} \tag{10.26g}$$

WHy all this? Add interactions $p^\mu \to p^\mu + eA^\mu$ or $i\not\partial \to i\not\partial + e\not A$

$$\mathcal{L} = \overline{\psi}\left(i\not\partial - m\right)\psi + eA_\mu\overline{\psi}\gamma^\mu\psi \tag{10.27a}$$

with

$$eA_\mu\overline{\psi}\gamma^\mu\psi = eA_\mu j^\mu \tag{10.27b}$$

recall (section 5)

$$\begin{aligned}
\hat{U} &= T\left(e^{-i\int_{t_0}^t \mathrm{d}t\,\hat{V}_\mathrm{I}(t)}\right) \\
&= \left(1 - i\int_{t_0}^t \mathrm{d}t\,\hat{V}_\mathrm{I} + \dots\right)
\end{aligned} \tag{10.27c}$$

recall section4, transition matrix elements $\langle f|\, \hat{U}\, |i\rangle$ with f and i having different particle content