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Skript

zur Vorlesung

Quantenmechanik II

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Inhaltsverzeichnis

1 Streutheorie

1. Spährisches Kastenpotential

$$V(r,\theta,\phi) = V(r) = \begin{cases} -V_0 & r < a \\ 0 & r \geq a \end{cases}$$

Mit der zeitabhängigen Schrödingergleichung: $i\hbar\frac{\partial\Psi}{\partial t}(\vec{x},t) = H\Psi(\vec{x},t)$
und dem Hamiltonoperator

$$H = \frac{\vec{p}^2}{2m} + V(r) = -\frac{\hbar^2}{2m}\Delta + V(r),$$

erhält man als Lösungen der zeitabhängigen Schrödingergleichung:

$$\Psi\vec{x},t = \psi x e^{-i\frac{E}{\hbar}t}$$

Wo bei für ψ gilt: $H\psi = E\psi$
Als Nächstes lösen wir die zeitunabhängige Schrödingergleichung in Kugelkoordinaten:

$$H = -\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\vec{L}}{2mr^2} + V(r)$$

Seperationsansatz:

$$\psi(r,\Theta,\phi) = R(r)Y_{lm}(\Theta,\phi)$$
$$\vec{L}^2 Y_{lm} = \hbar^2 l(l+1)Y_{lm}$$

einsetzen liefert:

$$\left(-\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{2}{r}\partial_r - \frac{l(l+1)}{r^2}\right) + V(r)\right)R(r)Y_{lm} = ER(r)Y_{lm}$$

$$\Leftrightarrow \left(\partial_r^2 + \frac{2}{r}\partial_r - \frac{l(l+1)}{r^2} + k^2\right)R(r) = 0 \quad \text{mit } k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$$

Substitution: $\rho = kr, \quad \partial_r = k\partial_\rho$

$$\Rightarrow \boxed{\left(\partial_\rho^2 + \frac{2}{\rho}\partial_\rho - \frac{l(l+1)}{\rho^2} + 1\right)R(\rho) = 0} (\star)$$

Dies ist die Bessel DGL; Lösen als Hausaufgabe.
Aufgabe 1: a) Ziegen sie, dass für $l = 0$ $\frac{\sin\rho}{\rho}, -\frac{\cos\rho}{\rho}$ Lösungen sind. b) Zeigen sie, dass $\rho^l\chi_l$ $(\star)$ erfüllt falls

$$\left(\partial_\rho^2 + \frac{2}{\rho}\partial_\rho - \frac{l(l+1)}{\rho^2} + 1\right)\chi_l = 0 \quad (\star\star)$$

c) Zeigen sie, dass $\chi_{l+1} := \frac{1}{\rho}\partial_\rho \chi_l$ die DGL ($\star\star$) für $(l+1)$ erfüllt, falls χ_l sie für l erfüllt.

$$j_l = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} : \qquad \text{(sphärische Besselfunktionen)}$$
$$n_l = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\cos\rho}{\rho} : \qquad \text{(sphärische Neumannfunktionen)}$$

Sowie die sphärischen Hantelfunktionen:

$$h_l^1 := j_l + in_l$$
$$n_l^2 := j_l - in_l = (n_l^1)^*$$

<u>Asymptotisches Verhalten:</u>

$$\rho \to 0: \quad j_l(\rho) \to \frac{\rho^l}{1\cdot 3\cdot 5\cdot ...\cdot(2l+1)}, \quad n_l(\rho) \leftarrow -\frac{1\cdot 3\cdot 5\cdot ...\cdot(2l+1)}{\rho^{l+1}}$$
$$\rho \to \infty: \quad j_l \to \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right), \quad n_l \to -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right)$$
$$h_l^1 \to \frac{1}{\rho}e^{i\left(\rho - \frac{l\pi}{2}\right)}$$
$$h_l^2 \to -\frac{1}{\rho}e^{-i\left(\rho - \frac{l\pi}{2}\right)}$$

<u>Gebundene Zustände:</u> $-V < E < 0$
Definition:

$$q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \quad \text{für } r < a$$
$$k = \sqrt{\frac{-2mE)}{\hbar^2}} \quad \text{für } r > a$$

Dann lautet die Bessel DGL:

$$\left(\partial_\rho^2 + \frac{2}{\rho}\partial_\rho - \frac{l(l+1)}{\rho^2} + \begin{pmatrix} q^2 \\ -k^2 \end{pmatrix}\right) R) = 0 \qquad \begin{matrix} r < a \\ r > a \end{matrix}$$

Randbedingungen:

$$
\begin{aligned}
R(r=0) \text{ ordentlich} &\Rightarrow R_l(r) = Aj_l(qr) \text{ für } 0 \leq r \leq a \\
\lim_{r\to\infty} R(r) \stackrel{!}{=} 0 \text{ ordentlich} &\Rightarrow R_l(r) = Aj_l(qr) \text{ für } a < r \\
&\Rightarrow A_{jl}(qa) = Bh_l^1(ika) \\
&\quad Aqj_l'(qa) = ikaBh_l'^1(ika) \\
&\Rightarrow \frac{Aqj_l(qa)}{Aj_l(qa)} = \frac{ikBh_l'^1(ika)}{Bh_l^1(ika)} \\
&\Leftrightarrow q\frac{d}{d\rho}ln(j_l)|_{\rho=aq} = ik\frac{d}{d\rho}ln(h_l^1)|_{\rho=ika}
\end{aligned}
$$

Berechnung für $l = 0$:

$$
\begin{aligned}
q\frac{d}{d\rho}ln\left(\frac{\sin\rho}{\rho}\right)|_{\rho=qa} &= ik\frac{d}{d\rho}ln\left(\frac{sin\rho - icos\rho}{\rho}\right)|_{\rho=ika} \\
\Leftrightarrow q\left(\cot(qa) - \frac{1}{qa}\right) &= -k - \frac{ik}{ika} \\
\Rightarrow \cot(qa) &= -\frac{k}{q}
\end{aligned}
$$

Streuzustände: $E > 0$

$$
R_l = \begin{cases} Aj_l(qr) & r < a \\ Bj_l(kr) + Cn_l(kr) & r > 0 \end{cases}
$$

$$
k = \sqrt{\frac{2mE}{\hbar^2}}, \quad q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}
$$

Randbedingungen:

$$
\begin{aligned}
Aj_l(qa) &= Bj_l(ka) + Cn_l(ka) \\
Aqj_l'(qa) &= k\left(Bj_l'(ka) + Cn_l'(ka)\right) \\
\lim_{r\to\infty} R_l &= \frac{B}{kr}\left(\sin(kr - \frac{l\pi}{2})\right) - \frac{C}{B}\cos\left(kr - \frac{l\pi}{2}\right) \\
&= \frac{B}{\cos\delta_l}\frac{1}{kr}\sin\left(kr - \frac{\pi}{2} + \delta_l\right) = R_l
\end{aligned}
$$

Mit der Phase: $\frac{C}{B} = -\tan\left(\delta_l(k)\right)$

2 Zwei spezielle Funktionen: Delta-Funktion und Greens-Funktionen

2.1 $\delta - Funktion$

Definition: $\delta_n(x) := \frac{1}{\pi}\frac{\frac{1}{n}}{x^2+\frac{1}{n^2}}$
Eigenschaften:

$$i) \lim_{n\to\infty} \delta_n(x) \begin{cases} \infty & x = 0 \\ 0 & sonst \end{cases}$$

$$ii) \lim_{n\to\infty} \int_\alpha^\beta dx \delta_n(x) f(x)$$
$$= \lim_{n\to\infty} \int_\alpha^\beta dx \frac{1}{\pi}\frac{\frac{1}{n}}{x^2+\frac{1}{n^2}} f(x)$$
$$\overset{sub.:x=\frac{y}{n}}{=} \lim_{n\to\infty} \int_{n\alpha}^{n\beta} dx \frac{1}{1+y^2} f\left(\frac{y}{n}\right) \qquad \alpha < 0, \beta > 0$$
$$= \lim_{n\to\infty} \int_{-\infty}^{+\infty} dx \frac{1}{1+y^2} f(0)$$
$$= f(0)$$

Dies gilt für alle f(x), welche für $\lim_{x\to\infty}$ schneller als $\frac{1}{x}$ gegen Null gehen.
Definition: Die Dirac'sche Delta-Distribution

$$\int_\alpha^\beta dx \delta(x) f(x) = \lim_{n\to\infty} \int_\alpha^\beta dx \delta_n(x) f(x)$$

Eigenschaften:

$$i) \int_{-\infty}^{+\infty} dx \delta(x) f(x) = f(0)$$
$$ii) \int_{-\infty}^{+\infty} dx \delta(x-a) f(x) = f(a)$$
$$iii) \int_{-\infty}^{+\infty} dx \delta'(x) f(x) = -\frac{df}{dx}|_{x=0}$$
$$iv) \delta(ax) = \frac{1}{|a|}\delta x$$

Definition: Die n-dimensionále Delta-Funktion
Mit $\vec{x} = \sum_{i=1}^{N} x_i \vec{e}_i, \quad \vec{a} = \sum_{i=1}^{N} a_i \vec{e}_i$

$$\delta^{(n)}(\vec{x} - \vec{a}) := \delta(x_1 - a_1)\delta(x_2 - a_2)...\delta(x_n - a_n)$$
$$\int_{-\infty}^{+\infty} dx^{(n)} \delta^{(N)}(vecx - \vec{a}) f(\vec{x}) = f(\vec{a})$$

Aufgabe 2:
a) Zeigen Sie ii)-iv)
b) Zeigen Sie, dass in Kugelkoordinaten gilt:

$$\delta^{(3)}(\vec{x} - \vec{x}') = \frac{1}{r^2}\delta(r - r')\delta(\cos\theta - \cos\theta')\delta(\phi - \phi')$$

Die Integraldarstellung der Delta-Funktion:
Fourier-Transformation von F(x):

$$\widetilde{F}(\omega) := \int_{-\infty}^{+\infty} dx e^{i\omega x} F(x)$$
$$F(x) := \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-i\omega x} \widetilde{F}(\omega)$$

Setzt man dies ineinander ein, folgt:

$$\begin{aligned} F(x) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-i\omega x} \int_{-\infty}^{+\infty} dy e^{i\omega y} F(y) \\ &= \int_{-\infty}^{+\infty} dy F(y) \underbrace{\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{i\omega(y-x)}}_{\delta(x-y)} \\ &\Rightarrow \boxed{\delta(x-y) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{i\omega(y-x)}} \end{aligned}$$

2.2 Greens-Funktionen

Gegeben sie die lineare Differentialgleichung: $D_x\psi(x) = f(x)$
Definition: Greens-Funktion $G(x - x')$

$$D_x G(x - x') = \delta(x - x')$$

Behauptung:

$$\psi(x) = \psi_{\text{hom}} + \int dx' G(x - x') f(x'), \qquad D_x \psi_{\text{hom}} = 0$$

Beweis:

$$D_x\left(\psi_{\text{hom}}+\int dx' G(x-x')f(x')\right)=\int dx' \underbrace{D_x G(x-x')}_{\delta(x-x')}f(x')=f(x)$$

<u>Anwendung:</u>
i) Poisson-Gleichung

$$\Delta\phi=\rho(x),\quad \vec{E}=-\vec{\nabla}\phi\Rightarrow G\sim\frac{1}{|\vec{x}-\vec{x}'|}$$

II) Umschreiben der Schrödingergleichung in eine Integralgleichung

$$\left(-\frac{\hbar^2}{2m}\Delta+V\right)\psi=E\psi$$

$$\Leftrightarrow\left(\Delta+k^2\right)\psi=\underbrace{\frac{2mV}{\hbar^2}\psi}_{\equiv f(x)},\qquad k=\frac{2mE}{\hbar^2}$$

$$\Rightarrow\boxed{\psi(\vec{x})=\psi_{hom}+\int d^3\vec{x}' G(\vec{x}-\vec{x}')\left(\frac{2mV}{\hbar^2}\right)\psi}$$

Mit $D_{\vec{x}}G(\vec{x}-\vec{x}')=\delta^{(N)}(\vec{x}-\vec{x}')$

<u>Finden der Greens-Funktion G:</u>

$$G(\vec{x}-\vec{x}')=\int\frac{d^3q}{(2\pi)3}\phi(\vec{q})e^{i\vec{q}(\vec{x}-\vec{x}')}$$

$$\left(\Delta+k^2\right)G(\vec{x}-\vec{x}')=\delta^{(3)}(\vec{x}-\vec{x}')$$

$$\Delta G=\int\frac{d^3q}{(2\pi)3}\phi(\vec{q})\Delta_{\vec{x}}e^{i\vec{q}(\vec{x}-\vec{x}')}$$

$$=\int\frac{d^3q}{(2\pi)3}\phi(\vec{q})(-\vec{q}^2)\vec{x}e^{i\vec{q}(\vec{x}-\vec{x}')}$$

$$\Rightarrow\left(\Delta_{\vec{x}}+k^2\right)G(\vec{x}-\vec{x}')=\int\frac{d^3q}{(2\pi)3}\phi(\vec{q})(q^2+k^2)\vec{x}e^{i\vec{q}(\vec{x}-\vec{x}')}$$

$$\stackrel{!}{=}\delta(\vec{x}-\vec{x}')=\int\frac{d^3q}{(2\pi)^3}e^{i\vec{q}(\vec{x}-\vec{x}')}$$

$$\Rightarrow\phi(\vec{q})=\frac{1}{k^2-q^2}$$

$$G(\vec{x}-\vec{x}')=\int\frac{d^3q}{(2\pi)^3}\frac{e^{i\vec{q}(\vec{x}-\vec{x}')}}{k^2-q^2}$$

Integration: Kugelkoordinaten $\vec{q} = (q, \theta, \phi)$
und mit $\vec{q}(\vec{x} - \vec{x}') = |\vec{q}||\vec{x} - \vec{x}'| \cos\theta$

$$\begin{aligned}
G(\vec{x} - \vec{x}') &= \frac{1}{(2\pi)^3} \int_0^\infty \frac{d^3q \cdot q^2}{k^2 - q^2} \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi e^{i\vec{q}(\vec{x}-\vec{x}')} \cdot \cos\theta \\
&= \frac{1}{(2\pi)^3} \int_0^\infty \frac{d^3q \cdot q^2}{k^2 - q^2} \left(2\pi \frac{e^{iq|\vec{x}-\vec{x}'|\cos\theta}}{iq|\vec{x} - \vec{x}'|} \right) |_{-1}^{+1} \\
&= \frac{1}{4\pi^2} \frac{1}{i|\vec{x} - \vec{x}'|} \int_0^\infty dq \frac{q}{k - q^2} \left(e^{iq|\vec{x}-\vec{x}'|} - e^{-iq|\vec{x}-\vec{x}'|} \right) \\
G(\vec{x} - \vec{x}') &= \frac{1}{4\pi^2} \frac{1}{i|\vec{x} - \vec{x}'|} \left(\int_0^\infty dq \frac{q}{k - q^2} e^{iq|\vec{x}-\vec{x}'|} - \int_{-\infty}^{0} dq \frac{q}{k - q^2} e^{iq|\vec{x}-\vec{x}'|} \right) \\
G(\vec{x} - \vec{x}') &= \frac{1}{4\pi^2} \frac{1}{i|\vec{x} - \vec{x}'|} \int_{-\infty}^{\infty} dq \frac{q}{k - q^2} e^{iq|\vec{x}-\vec{x}'|}
\end{aligned}$$

Komplexifizieren wir q und Integrieren im Komplexen können wir den Residuensatz benutzen. Es gibt vier mögliche Wege wie wir um die Pole$(k, -k)$ integrieren k"0nnen:
1) Integration bei Auslassung beider Pole
2) Integration bei Mitnahme des Pols bei k.
3) Integration bei Mitnahme des Pols bei -k.
4) Integration bei Mitnahme beider Pole.
Wir erhalten 4 verschiedene Greens-Funktionen:

$$1) G = 0$$

$$2) G_+ = \frac{1}{4\pi} \frac{1}{i|\vec{x} - \vec{x}'|} e^{ik|\vec{x}-\vec{x}'|}, \qquad \text{retardierte Greens-Funktion}$$

$$3) G_- = \frac{1}{4\pi} \frac{1}{i|\vec{x} - \vec{x}'|} e^{-ik|\vec{x}-\vec{x}'|}, \qquad \text{avancierte Greens-Funktion}$$

$$4) G = G_+ + G_-$$

Die Residuen erhält man aus der Gleichung:

$$\frac{1}{2\pi i} \oint_o dz f(z) = c_{-1}$$

Mit dem Entwicklungskoeffizient der Laurent-Reihe c_{-1} des $\frac{1}{z-q}$-Terms der Funktion $f(z)$.

3 Partial Wave Amplitude and Examples

BY SEBASTIAN JAKOBS

In scattering there are three different areas, in which we need to solve the Schrödinger-equation (SE): In the beginning we have the free initial state $\psi_0(t, \mathbf{x})$, then there is the interaction region, and finally the final state, which is also a free state. The initial state can be written as

$$\Psi_0(t, \mathbf{x}) = \int d^3k e^{i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{k}) \tag{3.1}$$

Last time we transformed the SE into an integral-equation

$$\psi_{\mathbf{k}}(\mathbf{x}) = \psi_{hom} + \int d^3x' G(\mathbf{x} - \mathbf{x}') \frac{2mV}{\hbar^2} \psi(\mathbf{x}) \tag{3.2}$$

where ψ_{hom} solves the free SE $(\Delta + k^2)\psi_{hom} = 0$. G(**x**-**x**') is the Green's function

$$(\Delta + k^2) G(\mathbf{x} - \mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}') \tag{3.3}$$

We showed, that the Green's function can be written as

$$G(\mathbf{x} - \mathbf{x}') = (2\pi)^{-3} \int d^3q e^{i\mathbf{q}\cdot\mathbf{x}} \frac{1}{k^2 - q^2} \tag{3.4}$$

$$= \frac{1}{4\pi^2} \frac{1}{i|\mathbf{x} - \mathbf{x}'|} \int_{-\infty}^{\infty} dq \underbrace{\frac{q}{k^2 + q^2}}_{pole\,at\,q=\pm k} e^{i|\mathbf{q}||\mathbf{x}-\mathbf{x}'|} \tag{3.5}$$

Using the residue-theorem we obtained four different solutions for G. Two of them corresponding to wave-packets propagating forward in time (G_+) and backward (G_-)

$$G_\pm = -\frac{1}{4\pi} \frac{1}{\mathbf{x} - \mathbf{x}'} e^{\pm ik|\mathbf{x}-\mathbf{x}'|} \tag{3.6}$$

We now assume a short-range potential $V = 0$ for $|\mathbf{x}| > R$, and expand in $\frac{\mathbf{x}'}{\mathbf{x}} << 1$:

$$|\mathbf{x} - \mathbf{x}'| = \sqrt{\mathbf{x}^2 - 2\mathbf{x}\cdot\mathbf{x}' + \mathbf{x}'^2} \tag{3.7}$$

$$= |\mathbf{x}| \sqrt{1 - 2\frac{\mathbf{x}\cdot\mathbf{x}'}{\mathbf{x}^2} + \frac{\mathbf{x}'^2}{\mathbf{x}^2}} \tag{3.8}$$

$$\approx |\mathbf{x}| \left(1 - \frac{\mathbf{x}\cdot\mathbf{x}'}{\mathbf{x}^2}\right) \tag{3.9}$$

inserting into (3.2) gives:

$$\psi_{\mathbf{k}} = \psi_{hom} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3x' \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{x}-\mathbf{x}'|}V(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x}') \tag{3.10}$$

$$\approx e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}f_k(\theta,\varphi) \tag{3.11}$$

$$f_k(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int d^3x' e^{-ik\frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}|}}V(\mathbf{x}')\psi_k(\mathbf{x}') \tag{3.12}$$

ψ_k is a solution for one particular $\mathbf{k}$. The solution for a momentum-distribution (localized around $\mathbf{k}_0$) is:

$$\psi = \psi_0 + \frac{f_{\mathbf{k}_0}(\theta,\varphi)}{|\mathbf{x}}|\hat{\psi}_0(\mathbf{k}_0,|\mathbf{x}|) \tag{3.13}$$

$$\hat{\psi}_0 = (2\pi)^{-3}\int d^3k a(\mathbf{k})e^{i|\mathbf{k}||\mathbf{x}|} \tag{3.14}$$

In the last semester we introduced the differential cross section:

$$\frac{d\sigma}{d\Omega} = \frac{1}{N_{in}}\frac{dN(\Omega)}{d\Omega} \tag{3.15}$$

N_{in}: Number of incoming particles
dN: Number of particles scattered in $d\Omega$ around Ω
The total cross section σ is:

$$\sigma = \int \frac{d\sigma}{d\Omega}d\Omega \tag{3.16}$$

and the number of incoming particles can be obtained by

$$N_{in} = \int dt|\mathbf{j}_{in}| \tag{3.17}$$

$$\mathbf{j}_{in} = \frac{\hbar}{2mi}\left(\psi_0^*\nabla\psi_0 - \psi_0\nabla\psi_0^*\right) \tag{3.18}$$

$$\approx \frac{\hbar\mathbf{k}_0}{m}|\psi_0|^2 \tag{3.19}$$

where $\mathbf{j}_i$ is the incoming current. In the last step we approximated $\mathbf{j}_{in}$ by using that ψ_0 is peaked arround $\mathbf{k}_0$. The radial component of the outgoing current is:

$$j_r^{out} = \frac{\hbar}{2mi}\left(\psi_{out}^*\partial_r\psi_{out} - \psi_{out}\partial_r\psi_{out}^*\right) \tag{3.20}$$

$$= \frac{\hbar\mathbf{k}_0}{m}\frac{1}{r^2}|f_{k_0}|^2|\psi_0|^2 \tag{3.21}$$

$$\rightarrow dN(\Omega) = \int dt j_r r^2 d\Omega \tag{3.22}$$

$$= \frac{\hbar k_0}{m}|f_{k_0}|^2 d\Omega \int dt|\psi_0|^2 \tag{3.23}$$

$$\tag{3.24}$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{\frac{\hbar k_0}{m}|f_{k_0}|^2 d\Omega \int dt|\psi_0|^2}{\frac{\hbar k_0}{m}\int dt|\psi_0|^2 d\Omega} = |f_{k_0}|^2 \tag{3.25}$$

Now we want to expand the exponentialfactor $e^{i\mathbf{k}\cdot\mathbf{x}}$ into orthogonal functions

$$e^{i\mathbf{k}\cdot\mathbf{x}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \hat{c}_{lm}(\mathbf{k}, r)Y_{lm}(\theta,\varphi) \tag{3.26}$$

choose a coordinates such that $\mathbf{k} = k\cdot\mathbf{e}_z$. Without loss of generality (w.l.o.g) we obtain

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} c_l(k,r)P_l(\cos\theta) \tag{3.27}$$

In Problem 4 is shown that:

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l(2l+1)j_l(kr)P_l(\cos\theta) \tag{3.28}$$

Important to note here is that, because most potentials don't depend on φ we do not need to concern ourselves with any φ-dependence in out expansion.

$$f_{|\mathbf{k}_0|} = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta) \tag{3.29}$$

$$\psi_k(r,\theta) = \sum_{l=0}^{\infty} i^l(2l+1)R_l(r)P_l(\cos\theta) \tag{3.30}$$

f_l is the partial wave amplitude

$$\psi_k \overset{r\to\infty}{=} \sum_l i^l(2l+1)\frac{P_l(\cos\theta)}{2ikr}\left(e^{i\left(kr-\frac{l\pi}{2}\right)} - e^{-i\left(kr-\frac{l\pi}{2}\right)}\right) \tag{3.31}$$

$$R_l = B_l j_l(kr) + C_l n_l(kr) \tag{3.32}$$

The Hankel-functions were introduced as

$$h_l^1 = j_l + in_l \tag{3.33}$$

$$h_l^2 = \left(h_l^1\right)^* \tag{3.34}$$

with these we can rewrite R_l

$$R_l = \left(h_l^2(kr) + S_l h_l^1(kr)\right) \tag{3.35}$$

In the last semester we showed, that for elastic scattering

$$j_r^{in} + j_r^{out} = 0 \tag{3.36}$$

this imposes a condition on S_l

$$|S_l|^2 = 1 \rightarrow S_l = e^{2i\delta_l} \tag{3.37}$$

all this gives us for ψ_k

$$\begin{aligned} \psi_k &= \sum_{l=0}^{\infty} i^l(2l+1)B_l\left(h_l^1(kr) + e^{2i\delta_l}h_l^1(kr)\right)P_l(\cos\theta) && (3.38)\\ &\overset{!}{=} \underbrace{e^{ikr\cos\theta}}_{\sum_{l=0}^{\infty} i^l(2l+1)j_l P_l} + \frac{e^{ikr}}{r} \underbrace{f_{12}}_{\sum_l (2l+1) f_l P_l} && (3.39) \end{aligned}$$

and

$$j_l = \frac{1}{2}\left(h_l^1 + h_l^2\right) \tag{3.40}$$

the comparison gives

$$\Rightarrow B_l = \frac{1}{2} \tag{3.41}$$

Left over is the condition

$$\frac{1}{2}\left(e^{2i\delta_l} - 1\right)h_l^1 = (-i)^l \frac{e^{ikr}}{r} f_l \tag{3.42}$$

which lets us compute the coefficients f_l of the expansion of the radial-wave part. Finally we study these coefficients in the asymptotic region

$$r \rightarrow \infty \quad h_l^1 \rightarrow -\frac{i}{kr}e^{i\left(kr - \frac{l\pi}{2}\right)} = \frac{1}{ikr}e^{ikr}\underbrace{e^{-i\frac{l\pi}{2}}}_{(-i)^l} \tag{3.43}$$

$$\rightarrow \frac{1}{2}\left(e^{2i\delta_l} - 1\right)\cdot\frac{1}{ikr}e^{ikr}(-i)^l = (-i)^l\frac{e^{ikr}}{r}f_l \tag{3.44}$$

Thus in the asymptotic region we find:

$$r \rightarrow \infty \quad f_l \rightarrow \frac{1}{2ik}\left(e^{2i\delta_l} - 1\right) \tag{3.45}$$

Summary In partial-wave analysis we can write the wave-function for one particular momentum as

$$\psi_{\mathbf{k}} = e^{ikz} + \frac{e^{ikr}}{r} f_k(\theta) \tag{3.46}$$

$$= \sum_{l=0}^{\infty} i^l (2l+1) R_l(kr) P_l(\cos\theta) \tag{3.47}$$

$$f_k = -\frac{m}{2\pi\hbar^2} \int d^3x' e^{-ik\frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}|}} V(\mathbf{x})\psi(\mathbf{x}) \tag{3.48}$$

$$= \sum_{l=0}^{\infty} i^l (2l+1) f_l P_l(\cos\theta) \tag{3.49}$$

$$R_l(kr) = \frac{1}{2}\left(h_l^2(kr) + e^{2i\delta_l} h_l^1(kr)\right) \tag{3.50}$$

There was also used the cylindrical symmetry of the problem, we assumed no φ-dependence. And finally

$$r \to \infty : \quad f_l = \frac{1}{2ik}\left(e^{2i\delta_l} - 1\right) = \frac{1}{k} e^{i\delta_l} \sin\delta_l \tag{3.51}$$

Another interesting question is the cross-section because it can be obseved by the experiment, thus the chief end of this analysis was the computation of the cross-section for one particular potential. Starting from the relation between differential cross-section and the partial-wave amplitude we find (for $r \to \infty$):

$$\frac{d\sigma}{d\Omega} = |f_k|^2 = \frac{1}{k^2}\left(\sum_{l=0}^{\infty}(2l+1)\sin\delta_l e^{i\delta_l} P_l(\cos\theta)\right)\cdot\left(\sum_{l'=0}^{\infty}(2l'+1)\sin\delta_{l'} e^{-i\delta_{l'}} P_{l'}(\cos\theta)\right)$$

$$= \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)\sin\delta_l \sin\delta_{l'} e^{i(\delta_l-\delta_{l'})} P_l(\cos\theta) P_{l'}(\cos\theta)$$

And finally for the total cross-section:

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin\delta_l \tag{3.52}$$

where we used the orthogonality of the Legendre-Polynominals

$$\int d\Omega P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{4\pi}{2l+1}\delta_{ll'} \tag{3.53}$$

So far we are not able to compute f_k since we still lack a first approximation of $\psi(x)$. This is done in the **Born-approximation** where we set $\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$:

$$\begin{aligned} f_k &= -\frac{m}{2\pi\hbar^2}\int d^3x' e^{-ik\frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}|}} V(\mathbf{x}')\psi(\mathbf{x}') && (3.54) \\ &= -\frac{m}{2\pi\hbar^2}\int d^3x' e^{i(\mathbf{k}-k\frac{\mathbf{x}}{|\mathbf{x}|})\cdot\mathbf{x}'} V(\mathbf{x}') && (3.55) \end{aligned}$$

Thus f_k is the Fourier-transform of the Potential.

3.1 Hard sphere

As a first example we will study a hard sphere of radius a.
We expanded ψ in Legendre-Polynominals (3.47) where the r-dependence is contained in $R_l(kr)$:

$$\begin{aligned} R_l(kr) &= \frac{1}{2}\left(h_2^l(kr) + e^{2i\delta_l} h_l^1(kr)\right) && (3.56) \\ &= e^{i\delta_l}\left(j_l \cos\delta_l - n_l \sin\delta_l\right) && (3.57) \end{aligned}$$

Since the spehere is hard, the amplitude ψ must vanish for $r \leq a$:

$$R(ka) = 0 \qquad (3.58)$$

$$\begin{aligned} \leftrightarrow j_l \cos\delta_l &= n_l \sin\delta_l && (3.59) \\ \cot\delta_l &= \frac{n_l(ka)}{j_l(ka)} && (3.60) \\ &\stackrel{k\to 0}{\to} \frac{(ak)^{-(l+1)}}{(ak)^l} = (ak)^{-(2l+1)} && (3.61) \\ \tan\delta_l &\to (ak)^{2l+1} && (3.62) \end{aligned}$$

From this we can conclude that in the expansion of $\frac{d\sigma}{s\Omega}$

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)\sin\delta_l \sin\delta_{l'} e^{i(\delta_l-\delta_{l'})} P_l(\cos\theta)P_{l'}(\cos\theta) \qquad (3.63)$$

the leading term for $k \to 0$ will be $l = 0$. This is also called s-wave-scattering

$$\begin{aligned} \frac{d\sigma}{d\Omega} &\stackrel{k\to 0}{\to} \frac{1}{k^2}\sin^2\delta_0 && (3.64) \\ \tan\delta_0 &\approx ak && (3.65) \end{aligned}$$

In first order approximation $\sin\delta_0 \approx \tan\delta_0$. This finally gives us

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \overset{k\to 0}{\to} \frac{4\pi}{k^2}\sin^2\delta_0 \tag{3.66}$$

$$= \frac{4\pi}{k^2}(ak)^2 = 4\pi a^2 \tag{3.67}$$

which is precisely the result of the analysis in classical mechanics.

3.2 Square well

The other example is the square well potential

$$V(r) = \begin{cases} 0, & r \geq a \\ -V_0, & r < a \end{cases} \tag{3.68}$$

Outside the well we have waves which must vanish for $r \to \infty$ and inside we have waves wich must be regular for $r \to 0$:

$$r > a, \quad R_l^{>}(kr) = e^{i\delta_l}\left(j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l\right) \tag{3.69}$$

$$r < a, \quad R_l^{<}(qr) = Aj_l(qr) \tag{3.70}$$

note that these to wave parts depend on different momenta

$$k = \frac{\sqrt{2mE}}{\hbar} \tag{3.71}$$

$$q = \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{3.72}$$

since the energy in the well is negative. The boundary conditions now read as:

$$Aj_l(qa) = R_l^{>}(ka) \tag{3.73}$$

$$A\frac{dj_l}{dr}(qr)\bigg|_{r=a} = \frac{d}{dr}R_l^{>}(kr)\bigg|_{r=a} \tag{3.74}$$

Dividing these two conditions by eachother we get

$$\alpha = \frac{1}{R_l^{>}(kr)}\frac{dR_l^{>}}{dr}(kr)\bigg|_{r=a} = \frac{1}{j_l(qr)}\frac{dj_l}{dr}(qr)\bigg|_{r=a} \tag{3.75}$$

$$= \frac{e^{i\delta_l}\left(\frac{dj_l}{dr}(kr)\cos\delta_l - \frac{dn_l}{dr}(kr)\right)\big|_{r=a}}{e^{i\delta_l}\left(j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l\right)\big|_{r=a}} \tag{3.76}$$

$$\leftrightarrow \alpha_q \left(j_l \cos\delta_l - n_l \sin\delta_l\right)\big|_{r=a} = \left(\frac{dj_l}{dr}(kr)\cos\delta_l - \frac{dn_l}{dr}(kr)\sin\delta_l\right)\bigg|_{r=a} \quad (3.77)$$

$$\cos\delta_l \left(\alpha_q j_l(kr) - \frac{dj_l}{dr}(kr)\right)\bigg|_{r=a} = \sin\delta_l \left(\alpha_q n_l(kr) - \frac{dn_l}{dr}(kr)\right)\bigg|_{r=a} \quad (3.78)$$

$$\cot\delta_l = \left.\frac{\alpha_q n_l(kr) - \frac{dn_l}{dr}(kr)}{\alpha_q j_l(kr) - \frac{dj_l}{dr}(kr)}\right|_{r=a} \quad (3.79)$$

For small momenta we have the followiong behviour:

$$j_l(ka) \stackrel{k\to 0}{\to} (ka)^l \quad (3.80)$$

$$\frac{dj_l}{dr}(ka) \stackrel{k\to 0}{\to} l k^l a^{l-1} \quad (3.81)$$

$$n_l(ka) \stackrel{k\to 0}{\to} (ka)^{-(l+1)} \quad (3.82)$$

$$\frac{dn_l}{dr}(ka) \stackrel{k\to 0}{\to} -(l+1)k^{-(l+1)}a^{-(l+2)} \quad (3.83)$$

This gives us finally

$$\cot\delta_l \stackrel{k\to 0}{\to} \frac{\alpha_q k^{-(l+1)}a^{-(l+1)} + (l+1)k^{-(l+1)}a^{-(l+2)}}{\alpha_q k^l a^l - l k^l a^{l-1}} \quad (3.84)$$

$$= k^{-(2l+1)}a^{-(2l+1)}\frac{\alpha_q + (l+1)\frac{1}{a}}{\alpha_q - \frac{l}{a}} \quad (3.85)$$

$$\tan\delta_l \stackrel{k\to 0}{\to} (ak)^{2l+1}\frac{l - \alpha_q a}{l+1+\alpha a} \quad (3.86)$$

$$= -\frac{\gamma(ka)^{2l+1}}{E - E_R} \quad (3.87)$$

With this result we can compute the total cross-section

$$\sigma = \sum_l \sigma_l \qquad \sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l \quad (3.88)$$

$$\sin^2\delta_l = \frac{\tan^2\delta_l}{1+\tan\delta_l} = \frac{(\gamma(ka)^{2l+1})^2}{(E-E_R)^2}\frac{1}{1+\frac{(\gamma(ka)^{2l+1})^2}{(E-E_R)^2}} \quad (3.89)$$

$$= \frac{(\gamma(ka)^{2l+1})^2}{(E-E_R)^2 + (\gamma(ka)^{2l+1})^2} \quad (3.90)$$

This is also known as the Breit-Wigner-Formula. The qualitative form of that formula can be seen in Fig. 1

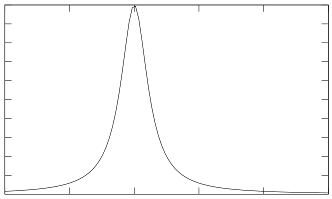

Abbildung 1: The qualitative behaviour of the Breit-Wigner-Formula

Further we can compute the partial-wave amplitudes:

$$
\begin{aligned}
f_l &= \frac{1}{k} e^{i\delta_l} \sin\delta_l = \frac{1}{k} \frac{\tan\delta_l}{1 - i\tan\delta_l} && (3.91) \\
&= -\frac{\gamma(ka)^{2l+1}}{k} \frac{1}{E - E_R + i\gamma(ka)^{2l+1}} && (3.92) \\
&= -\frac{\gamma}{k}(ka)^{2l+1} \frac{1}{E - E_R + i\gamma(ka)^{2l+1}} && (3.93)
\end{aligned}
$$

4 Non-relativistic many-particle system

By: Jasper Hasenkamp

4.1 N identical particles in quantum mechanics

The situation should be remembered for **one particle** with the Hamiltonian:

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x}, \vec{s}, \dots) = -\frac{\hbar^2}{2m}\Delta + V \tag{4.1}$$

The Schrödinger equation is:

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

if $\frac{\partial H}{\partial t} = 0$

$$\Rightarrow |\psi\rangle = \sum_i c_i e^{-\frac{iE_i}{\hbar}t}|i\rangle,\ H|i\rangle = E|i\rangle \tag{4.3}$$

The are

$$\{|i\rangle\} \epsilon \mathcal{H}$$

and the elements of the dual space $\mathcal{H}^*$ to the Hilbert space $\mathcal{H}$ then are

$$\{\langle i|\} \epsilon \mathcal{H}^*$$

with the known map

$$\langle\cdot|\cdot\rangle : \mathcal{H}^* \otimes \mathcal{H} \to \mathbb{C}$$

while the $|i\rangle$ are orthonormal, so that

$$\langle i|j\rangle = \delta_{ij}$$

in position space:

$$\int d^3x\, \psi_i^*(\vec{x})\psi_j(\vec{x}) = \delta_{ij}$$

With **N particles** the hamiltonian is:

$$H = \sum_{\alpha=1}^{N} \frac{\vec{p}_\alpha^2}{2m_\alpha} + V(\vec{x}_1, \vec{s}_1, \vec{x}_2, \dots) \equiv H(1, \dots, N) \tag{4.4}$$

For identical particles(i.e. particles with the same mass, charge, spin, etc.) follows, that the Hamiltonian is symmetric under the exchange of two particles, i.e.

$$\Rightarrow H(1, \dots, \alpha, \dots, \beta, \dots, N) = H(1, \dots, \beta, \dots, \alpha, \dots, N) \tag{4.5}$$

but the state is not: $|\psi\rangle = |1, \dots, N\rangle$

4.2 Introduction of the Permutation operator $P_{\alpha\beta}$

The Permutation operator $P_{\alpha\beta}$ interchanges $\alpha \leftrightarrow \beta$.

$$P_{\alpha\beta}|1, \dots, \alpha, \dots, \beta, \dots, N\rangle = |1, \dots, \beta, \dots, \alpha, \dots, N\rangle \tag{4.6}$$

Properties:

(i) $P^2 = 1 \Rightarrow$ Eigenvalues of P are ± 1

(ii) (under the assumption of identical particles)
$PH = HP \Rightarrow P|\psi\rangle$ has same Eigenvalues as $|\psi\rangle$
Proof: $H(P|\psi\rangle) = PH|\psi\rangle = PE|\psi\rangle = E(P|\psi\rangle)$

(iii) $\langle\varphi|\psi\rangle = \langle P\varphi|P\psi\rangle$

$$\begin{aligned} \Leftrightarrow \quad & \int d^3x_1 \dots d^3x_N\, \varphi^*(\vec{x}_1, \dots, \vec{x}_\alpha, \dots, \vec{x}_\beta, \dots, \vec{x}_N)\psi(\vec{x}_1, \dots, \vec{x}_\alpha, \dots, \vec{x}_\beta, \dots, \vec{x}_N) \\ = \quad & \int d^3x_1 \dots d^3x_N\, \varphi^*(\vec{x}_1, \dots, \vec{x}_\beta, \dots, \vec{x}_\alpha, \dots, \vec{x}_N)\psi(\vec{x}_1, \dots, \vec{x}_\beta, \dots, \vec{x}_\alpha, \dots, \vec{x}_N) \\ = \quad & \langle\varphi|\psi\rangle \end{aligned}$$

, because the names of the indices do not change anything.

(iv) $P^\dagger = P^{-1} \Leftrightarrow P^\dagger P^{-1} = \underline{1} \Leftrightarrow P$ is unitary
Proof:

$$\langle\varphi|P\psi\rangle = \langle P^\dagger\varphi|\psi\rangle$$

via definition of $P^\dagger$. With (iii) it is equal to

$$\langle P^{-1}\varphi|P^{-1}P\psi\rangle = \langle P^{-1}\varphi|\underline{1}\psi\rangle = \langle P^{-1}\varphi|\psi\rangle$$

(v) With a symmetric operator S: $S(1, \dots, \alpha, \dots, \beta, \dots, N) = S(1, \dots, \beta, \dots, \alpha, \dots, N)$ (for example H) the commutator vanishes $\Rightarrow [P, S] = 0$ and

$$\langle P\psi_i|S|P\psi_j\rangle = \langle\psi_i|P^\dagger SP|\psi_j\rangle = \langle\psi_i|P^\dagger PS|\psi_j\rangle = \langle\psi_i|S|\psi_j\rangle$$

There are two **different types of particles**:

Bosons: $P_{\alpha\beta}|\psi_s\rangle = |\psi_s\rangle \;\forall\alpha, \beta$

Fermions: $P_{\alpha\beta}|\psi_a\rangle = -|\psi_a\rangle \;\forall\alpha, \beta$

For **example**: two particles

$$|\psi_s\rangle = \tfrac{1}{\sqrt{2}}(|1,2\rangle + |2,1\rangle)$$
$$|\psi_a\rangle = \tfrac{1}{\sqrt{2}}(|1,2\rangle - |2,1\rangle)$$

and three particles

$$|\psi_s\rangle = \tfrac{1}{\sqrt{6}}(|1,2,3\rangle + |2,3,1\rangle + |3,1,2\rangle + |2,1,3\rangle + |1,3,2\rangle + |3,2,1\rangle)$$
$$|\psi_a\rangle = \tfrac{1}{\sqrt{6}}(|1,2,3\rangle + |2,3,1\rangle + |3,1,2\rangle - |2,1,3\rangle - |1,3,2\rangle - |3,2,1\rangle)$$

This leads for N particles to:

$$|\psi_s\rangle = \tfrac{1}{\sqrt{N!}}\textstyle\sum_P P|1,2,\ldots,N\rangle \tag{4.7}$$
$$|\psi_a\rangle = \tfrac{1}{\sqrt{N!}}\textstyle\sum_P (-1)^P P|1,2,\ldots,N\rangle \tag{4.8}$$

Where P in the sum means to write down all (non-equal) permutations. See that

$$(-1)^P = \begin{cases} 1 & \textit{even Permutations} \\ -1 & \textit{odd Permutations} \end{cases} \tag{4.9}$$

<u>Now</u> the restriction to **non-interacting** particles has following effect:

$$H = \sum_{\alpha=1}^{N} H_\alpha,\ H_\alpha = \frac{\vec{p}_\alpha^{\,2}}{2m} + V(\vec{x}_\alpha) \tag{4.10}$$

$\Rightarrow$ Eigenstates

$$\mathcal{H} \ni |1,2,\ldots,N\rangle = |i_1\rangle_1 \otimes \ldots \otimes |i_N\rangle_N = \bigotimes_{\alpha=1}^{N} \mathcal{H}_\alpha$$

Where the index *in* the Ket denotes the state of the particle (1-particle Hamiltonian) and the index at the Ket itself denotes the particle. The $\mathcal{H}_\alpha$ are all equal.

$$\Leftrightarrow H_\alpha|i\rangle_\alpha = \in_i |i\rangle_\alpha \tag{4.11}$$

4.3 Occupation-number representation

One particle states appear with following multiplicities

state	$\|1\rangle$	n_1
	$\|2\rangle$	n_2
	$\|3\rangle$	n_3
	$\vdots$	$\vdots$

A logical constraint is, that

$$\sum_{i=1}^{\infty} n_i = N \tag{4.12}$$

It is, that the sum over the occupation numbers is the number of particles. You get by thinking:

$$n_i = \begin{cases} 0,1 & Fermions \\ 0,1,2,\ldots & Bosons \end{cases} \tag{4.13}$$

How many terms are in

$$\begin{array}{cc} |\psi_a\rangle & N! \\ |\psi_s\rangle & \frac{N!}{n_1!\,n_2!\cdots} \end{array}$$

Normalization:

$$1 = \langle\psi_a|\psi_a\rangle = \frac{1}{N!}\cdot N! = 1$$

It is used, that the states are normalized to 1 allready.

$$\langle\psi_s|\psi_s\rangle = \frac{1}{N!}(n_1!\cdot n_2!\cdots)^2\frac{N!}{n_1!\cdot n_2!\cdots} = n_1!\cdot n_2!\cdots \neq 1$$

Example:

$$|1,2,3\rangle = \frac{1}{\sqrt{6}}(|1,2,3\rangle + |2,3,1\rangle + |3,1,2\rangle + |2,1,3\rangle + |1,3,2\rangle + |3,2,1\rangle)$$

Now state 1 is equal to state 2. This gives:

$$\begin{aligned} &= \frac{1}{\sqrt{6}}(2|1,1,3\rangle + 2|1,3,1\rangle + 2|3,1,1\rangle) \\ &= \frac{2}{\sqrt{6}}(|1,1,3\rangle + |1,3,1\rangle + |3,1,1\rangle) \\ &= \frac{2!}{\sqrt{6}}(\ldots) = \frac{n_1!}{\sqrt{N!}}(\ldots) \end{aligned}$$

This leads to a new normalization term for $|\psi_s\rangle$

$$|\psi_s\rangle = \frac{1}{\sqrt{N!}}\frac{1}{\sqrt{n_1!n_2!\cdots}}\sum_P P(1,2,\ldots,N\rangle \tag{4.14}$$

5 Creation and annihilation Operators for Fermions

Definition By: `Sebastian Jakobs`
The fermionic many-particle state-vecor is

$$\begin{aligned} |n_1 n_2 ...\rangle &= \frac{1}{\sqrt{N!}} \sum_P (-1)^P P \, |i_1\rangle_1 \otimes ... \otimes |i_N\rangle_N \\ &= \frac{1}{\sqrt{N!}} \begin{vmatrix} |i_1\rangle_1 & ... & |i_1\rangle_N \\ \vdots & \ddots & \vdots \\ |i_N\rangle_1 & ... & |i_N\rangle_N \end{vmatrix} \end{aligned}$$

In the last equality the antisymetric sum was written as a **Slater-Determinant**. The Pauli-Exclusion-Principle states that a state can only be occupied by atmost one particle, therefore: $n_i = 0, 1$. E.g.:

$$|1, 0, 0, 1, ...\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle_1 |4\rangle_2 - |4\rangle_1 |1\rangle_2 \right) \tag{5.1}$$

The Ground-state $|0\rangle$ is the state with no particles. The vectors $|n_1 n_2 ...\rangle$ are Elements of Fock-Space, they are orthonormal to each other

$$\langle n_1' n_2' ... | n_1 n_2 ...\rangle = \delta_{n_1' n_1} \cdot \delta_{n_2' n_2} \cdot ... \tag{5.2}$$

A one-particle-state can be created by the action of a creation-operator

$$a_i^\dagger |0\rangle = |0, ..., 0, n_i = 1, 0, ...\rangle \tag{5.3}$$

Definition 1. *The **Ground-state** is defined by the action of the annihilation-operator*

$$a_i |0\rangle = 0 \quad \forall_i \tag{5.4}$$

An arbitrary many-particle-state can be created by

$$\left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} ... |0\rangle = |n_1 n_2 ...\rangle \tag{5.5}$$

The action of the annihilation-Operator a_i is given by

$$\begin{aligned} a_i |0\rangle &= 0 & (5.6) \\ a_i |0, ..., 0, n_i = 1, 0, ...\rangle &= |0\rangle & (5.7) \\ (a_i)^2 |...\rangle &= 0 & (5.8) \end{aligned}$$

The state-vector in the last equality is an arbitrary vector.

The action of the creation- and annihilation-Operators can be summarized by:

$$a_i^\dagger \left|n_1 n_2 ...\right\rangle = (1-n_i)\,(-1)^{\sum_{j<i} n_j} \left|n_1, ..., n_i+1, ...\right\rangle \tag{5.9}$$

$$a_i \left|n_1 n_2 ...\right\rangle = n_i (-1)^{\sum_{j<i} n_j} \left|n_1, ..., n_i-1, ...\right\rangle \tag{5.10}$$

From this we can conclude

$$\left\| a_i^\dagger \left|n_1 n_2 ...\right\rangle \right\|^2 = \langle ...|\, a_i a_i^\dagger \,|...\rangle = (1-n_i)(n_i+1)\left((-1)^{\sum_{j<i} n_j}\right)^2 \tag{5.11}$$

$$= 1 - n_i^2 = \begin{cases} 1 & n_i = 0 \\ 0 & n_i = 1 \end{cases} \tag{5.12}$$

Algebra of a and $a^\dagger$

- $\left(a_i^\dagger\right)^2 = (a_i)^2 = 0$
- $\left\{a_i^\dagger, a_j^\dagger\right\} = a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0$
- $\{a_i, a_j\} = 0$
- $\left\{a_i, a_j^\dagger\right\} \left|n_1 n_2 ...\right\rangle = \begin{cases} \left|n_1 n_2 ...\right\rangle & i = j \\ 0 & i \neq j \end{cases}$

N-particle-Operators can be written in terms of creation- and annihilation-Operators now. A **One-particle-Operator** is:

$$T = \sum_{\alpha=1}^{N} t_\alpha = \sum_\alpha \sum_{i,j} t_{ij} |i\rangle_\alpha \langle j|_\alpha \tag{5.13}$$

where

$$\sum_\alpha |i\rangle_\alpha \langle j|_\alpha = a_i^\dagger a_j \tag{5.14}$$

A **Two-particle-Operator** takes the form ($\alpha \neq \beta$):

$$F = \frac{1}{2} \sum_\alpha \sum_\beta f^{(2)}(\mathbf{x}_\alpha, \mathbf{x}_\beta) = \frac{1}{2} \sum_{i,j,k,m} \langle ij|f^{(2)}|km\rangle a_i^\dagger a_j^\dagger a_k a_m \tag{5.15}$$

5.1 Completenessrelation

Given tha $\varphi_i(\mathbf{x})$ is a basis of $\mathcal{H}_\alpha$, the one-particle Hilbert-space of particle α. Then an arbitrary state can be written as:

$$\psi(\mathbf{x}) = \sum_i c_i \varphi_i(\mathbf{x}) \tag{5.16}$$

$$c_i = \int d^3\mathbf{x} \varphi_i^*(\mathbf{x}\psi(\mathbf{x}) \tag{5.17}$$

From this follows

$$\psi(\mathbf{x}) = \int d^3\mathbf{x}' \psi(\mathbf{x}')\delta^{(3)}(\mathbf{x}-\mathbf{x}') = \sum_i c_i \int d^3\mathbf{x}' \varphi_i(\mathbf{x}')\delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{5.18}$$

$$= \sum_i \int d^3\mathbf{x}'' \varphi_i^*(\mathbf{x}'')\psi(\mathbf{x}'') \int d^3\mathbf{x}' \varphi_i(\mathbf{x}')\delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{5.19}$$

$$= \sum_i \int d^3\mathbf{x}'' \varphi_i^*(\mathbf{x}'')\varphi_i(\mathbf{x})\psi(\mathbf{x}'') \tag{5.20}$$

and hence the **Completenessrelation**

$$\sum_i \varphi_i^*(\mathbf{x}'')\varphi_i(\mathbf{x}) = \delta^{(3)}(\mathbf{x}''-\mathbf{x}) \tag{5.21}$$

6 Field operators

By: Sebastian Jakobs

Definition 2. ***Field Operator:***

$$\hat{\psi}(\boldsymbol{x}) := \sum_i \varphi_i(\boldsymbol{x}) a_i \tag{6.1}$$

where $\varphi_i(\boldsymbol{x})$ is a one-particle-wavefunction

The adjoint of this operator is given by

$$\hat{\psi}^\dagger(\mathbf{x}) = \sum_i \varphi_i^*(\mathbf{x}) a_i^\dagger \tag{6.2}$$

Both operator-definitions are valid for Bosons and Fermions. The commutation- and anticommutation-relations can be derived using those of a and $a^\dagger$.

$$\begin{aligned}
\left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}')\right]_\pm &= \sum_{i,j} \varphi_i(\mathbf{x})\varphi_j(\mathbf{x}') \left[a_i, a_j\right]_\pm & (6.3)\\
&= 0 & (6.4)\\
\left[\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\right]_\pm &= 0 & (6.5)\\
\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\right]_\pm &= \sum_{i,j} \varphi_i(\mathbf{x})\varphi_j^*(\mathbf{x}') \left[a_i, a_j^\dagger\right]_\pm & (6.6)\\
&= \sum_i \varphi_i(\mathbf{x})\varphi_i^*(\mathbf{x}') & (6.7)\\
&= \delta^{(3)}(\mathbf{x} - \mathbf{x}') & (6.8)
\end{aligned}$$

The physical interpretation of the field-operators: They create ($\hat{\psi}^\dagger$) or annihilate ($\hat{\psi}$) a particle at point $\mathbf{x}$.
What is the Hamiltonian expressed in terms of $\hat{\psi}^\dagger$ and $\hat{\psi}$?

$$H = \sum_{\alpha=1}^{N} \left(\frac{\mathbf{p}_\alpha^2}{2m} + V(\mathbf{x}_\alpha) \right) = \sum_{i,j} H_{ij} a_i^\dagger a_j \tag{6.9}$$

The Matrixelements H_{ij} can be computed using partial integration:

$$\begin{aligned}
H_{ij} &= \langle i|H|j\rangle = \int d^3\mathbf{x} \varphi_i^*(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x}) \right) \varphi_j(\mathbf{x}) & (6.10)\\
&= \int d^3\mathbf{x} \left\{ \frac{\hbar^2}{2m} (\nabla\varphi_i^*) \cdot (\nabla\varphi_j) + V\varphi_i^*\varphi_j \right\} & (6.11)\\
& & (6.12)
\end{aligned}$$

inserted into (6.9)

$$H = \sum_{i,j} \int d^3\mathbf{x} \left\{ \frac{\hbar^2}{2m} \left(\nabla \varphi_i^* a_i^\dagger \right) \cdot \left(\nabla \varphi_j a_j \right) + V \varphi_i^* \varphi_j a_i^\dagger a_j \right\} \tag{6.13}$$

$$= \int d^3\mathbf{x} \left\{ \frac{\hbar^2}{2m} \left(\nabla \hat{\psi}^\dagger(\mathbf{x}) \right) \cdot \left(\nabla \hat{\psi}(\mathbf{x}) \right) + V(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \right\} \tag{6.14}$$

The same computation can be done for a 2-particle-Operator:

$$F = \frac{1}{2} \sum_{i,j,k,m} \langle ij | f^{(2)}(\mathbf{x}_1, \mathbf{x}_2) | km \rangle a_i^\dagger a_j^\dagger a_k a_m \tag{6.15}$$

$$= \frac{1}{2} \sum_{i,j,k,m} \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \varphi_i^*(\mathbf{x}_1) \varphi_j^*(\mathbf{x}_2) f^{(2)}(\mathbf{x}_1, \mathbf{x}_2) \varphi_m(\mathbf{x}_1) \varphi_m(\mathbf{x}_2) a_i^\dagger a_j^\dagger a_k a_m \tag{6.16}$$

$$= \frac{1}{2} \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \hat{\psi}^\dagger(\mathbf{x}_1) \hat{\psi}^\dagger(\mathbf{x}_2) f^{(2)}(\mathbf{x}_1, \mathbf{x}_2) \hat{\psi}(\mathbf{x}_1) \hat{\psi}(\mathbf{x}_2) \tag{6.17}$$

The particle-density $n(\mathbf{x})$ where $N = \int d^3\mathbf{x} n(\mathbf{x})$ is:

$$n(\mathbf{x}) = \sum_{\alpha=1}^{N} \delta^{(3)}(\mathbf{x} - \mathbf{x}_\alpha) \tag{6.18}$$

$n(\mathbf{x})$ is a one-particle-operator, and hence follows:

$$n(\mathbf{x}) = \sum_{i,j} a_i^\dagger a_j \langle i | n | j \rangle = \sum_{i,j} a_i^\dagger a_j \int d^3\mathbf{y} \varphi_i^*(\mathbf{y}) \delta^{(3)}(\mathbf{x} - \mathbf{y}) \varphi_j(\mathbf{y}) \tag{6.19}$$

$$= \sum_{i,j} a_i^\dagger a_j \varphi_i^*(\mathbf{x}) \varphi_j(\mathbf{x}) \tag{6.20}$$

$$= \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \tag{6.21}$$

Operators in Heisenberg- and Schrödinger-picture The Operators O_S in the Schrödinger-picture have no time-dependence. They are related to the Heisenberg-operators by

$$O_H(\mathbf{x}, t) = e^{i\frac{H}{\hbar}t} O_S(\mathbf{x}) e^{-i\frac{H}{\hbar}t} \tag{6.22}$$

For the field-operators follows then:

$$\hat{\psi}_H(\mathbf{x}, t) = e^{i\frac{H}{\hbar}t} \hat{\psi}(\mathbf{x}) e^{-i\frac{H}{\hbar}t} \tag{6.23}$$

The time-evolution of the Heisenberg-field-operators are given by the known relation:

$$i\hbar \frac{\partial \hat{\psi}_H}{\partial t} = \left[\hat{\psi}_H, H \right]_\pm \tag{6.24}$$

and

$$\left[\hat{\psi}_H, H\right]_\pm = e^{i\frac{H}{\hbar}t}\left[\hat{\psi}, H\right]_\pm e^{-i\frac{H}{\hbar}t} \tag{6.25}$$

In the following we will compute this commutator

$$\left[\hat{\psi}, H\right] = \int d^3\mathbf{y}\left[\hat{\psi}(\mathbf{x}), \frac{\hbar^2}{2m}\left(\nabla\hat{\psi}^\dagger(\mathbf{y})\right)\cdot\left(\nabla\hat{\psi}(\mathbf{y})\right) + V(\mathbf{y})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\right]_\pm \tag{6.26}$$

$$= \int d^3\mathbf{y}\left\{\frac{\hbar^2}{2m}\sum_{i=1}^{3}\left[\hat{\psi}(\mathbf{x}), \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i}\right]_\pm + V(\mathbf{y})\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\right]_\pm\right\} \tag{6.27}$$

$$\left[\hat{\psi}(\mathbf{x}), \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i}\right]_\pm = \left[\hat{\psi}(\mathbf{x}), \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\right]_\pm \frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i} \mp \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\left[\hat{\psi}(\mathbf{x}), \frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i}\right]_\pm \tag{6.28}$$

$$= \left[\hat{\psi}(\mathbf{x}), \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\right]_\pm \frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i} \mp \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\frac{\partial}{\partial y^i}\underbrace{\left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y})\right]_\pm}_{=0} \tag{6.29}$$

$$= \left[\hat{\psi}(\mathbf{x}), \frac{\partial\hat{\psi}^\dagger(\mathbf{y})}{\partial y^i}\right]_\pm \frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i} \tag{6.30}$$

$$= \frac{\partial\hat{\psi}(\mathbf{y})}{\partial y^i}\frac{\partial}{\partial y^i}\delta^{(3)}(\mathbf{x}-\mathbf{y}) \tag{6.31}$$

$$\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\right]_\pm = \left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_\pm \hat{\psi}(\mathbf{y}) \mp \hat{\psi}^\dagger(\mathbf{y})\underbrace{\left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y})\right]_\pm}_{=0} \tag{6.32}$$

$$= \left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_\pm \hat{\psi}(\mathbf{y}) \tag{6.33}$$

And hence follows

$$\Big[\hat{\psi}(\mathbf{x}), H\Big]_{\pm} = \int d^3\mathbf{y} \left\{ \left(\frac{\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial \hat{\psi}(\mathbf{y})}{\partial y^i} \frac{\partial}{\partial y^i} \delta^{(3)}(\mathbf{x}-\mathbf{y}) \right) + V(\mathbf{y})\delta^{(3)}(\mathbf{x}-\mathbf{y})\hat{\psi}(\mathbf{y}) \right\} \tag{6.34}$$

$$= -\frac{\hbar^2}{2m}\Delta\hat{\psi}(\mathbf{x}) + V(\mathbf{x})\hat{\psi}(\mathbf{x}) \tag{6.35}$$

$$= \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x}) \right) \hat{\psi}(\mathbf{x}) \tag{6.36}$$

Transforming back to the Heisenberg-picture gives:

$$i\hbar \frac{\partial \hat{\psi}_H}{\partial t}(\mathbf{x}, t) = e^{i\frac{H}{\hbar}t} \left[\left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x}) \right) \hat{\psi}(\mathbf{x}) \right] e^{-i\frac{H}{\hbar}t} \tag{6.37}$$

$$= \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x}) \right) \hat{\psi}_H(\mathbf{x}) \tag{6.38}$$

Thus we have found, that the field-operators satisfy the one-particle Schrödinger-equation. Therfore the presented method of introducing field-operators is referred to as "second-quantization".

7 Nachtrag zu fermionischen Erzeugungs- und Vernichtungsoperatoren

Start: $|0\rangle$

$a_i^\dagger|0\rangle \equiv |0,0,...,n_i=1,...\rangle = |i\rangle$

$a_i^\dagger a_j^\dagger|0\rangle \equiv |0,0,...,n_i=1,...,n_j=1,...\rangle = \frac{1}{\sqrt{2}}\left(|i\rangle|j\rangle - |j\rangle|i\rangle\right), \qquad i \neq j$

$a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger$

$(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}...|0\rangle = |n_1,n_2,...\rangle = \frac{1}{\sqrt{N}}\sum_P (-1)^P P|i_1\rangle \otimes ... \otimes |ß_N\rangle \qquad N = \sum_i^\infty n_i$

$a_i|0\rangle = 0$

$a_i|0,...,n_i=1,...\rangle = |0\rangle$

$a_i a_j|0,...,n_i=1,...,n_j=1...\rangle = |0\rangle$

$a_i a_j = -a_j a_i$

$a_i^\dagger|n_1,n_2,...,n_i,...\rangle = (1-n_i)(-1)^{\sum_{j<i} n_j}|n_1,n_2,...,n_i+1,...\rangle$

adjungieren der Gleichung liefert:

$\langle n_1,...,n_i,...|a_i = (1-n_i)(-1)^{\sum_{j<i} n_j}\langle n_1,n_2,...,n_i+1,...|$

$$\Rightarrow a_i|n_1,...,n_i',...\rangle = \underbrace{\sum_{n_i=0}^{1}|n_1,...,n_i,...\rangle\langle...,n_i,...n_1}_{1}|a_i|n_1,...,n_i',...\rangle$$

$$= \sum_{n_i}|n_1,...,n_i,...\rangle(1-n_i)n_i'(-1)^{\sum_{j<i} n_j}\delta_{n_i+1,n_i'}$$

$$= |n_1,...,n_i',...\rangle\underbrace{(1-(n_i'-1))n_i'}_{=1 \text{ für } n_i'=1,\ 0 \text{ sonst}}(-1)^{\sum_{j<i} n_j}$$

$$\Rightarrow \boxed{a_i|n_1,...,n_i,...\rangle = n_i(-1)^{\sum_{j<i} n_j}|n_1,...,n_i-1,...\rangle}$$

8 II.5 Feldoperatoren im Impulsraum

$$\widehat{\Psi}^\dagger(\vec{x}) = \sum_i \varphi_i^*(\vec{x})a_i^\dagger$$

Wir betrachten ein System in einem Kasten mit dem Volumen $V = L_x L_y L_z$. Die Eigenfunktionen des Impulsoperators sind gegeben durch:

$$\widehat{\vec{p}}\varphi = -i\hbar\vec{\nabla}\varphi = \vec{p}\varphi$$

$$\boxed{\varphi_{\vec{k}}(\vec{x})} = \frac{1}{\sqrt{V}}e^{i\vec{k}\vec{x}}, \qquad \vec{\nabla}\varphi_{\vec{k}} = i\vec{k}\varphi_{\vec{k}}, \qquad \vec{p} = \hbar\vec{k}$$

Periodischen Randbedingngen liefern:

$$\varphi(x + L_x, y, z) = \varphi(x, y, z)$$
$$\varphi(x, y + L_y, z) = \varphi(x, y, z)$$
$$\varphi(x, y, z + L_z) = \varphi(x, y, z)$$
$$\Rightarrow e^{ik_x x} = e^{ik_y y} = e^{ik_z z} = 1 \Rightarrow \boxed{k_I = 2\pi\frac{m_I}{L_I}} \qquad m_I \in \mathbb{Z}$$

Nun drücken wir den Hamiltonoperator durch $\varphi_{\vec{k}}$

$$H = \sum_{\alpha=1}^{N}\frac{\vec{p}}{2m} + U(\vec{x}_\alpha) = \sum_{i,j}\langle i|H|j\rangle a_i^\dagger a_j$$

$$\text{Mit } \langle i|H|j\rangle = \int d^3x\varphi_{\vec{k}_i}^*\left(-\frac{\hbar^2\Delta}{2m} + U\right)\varphi_{\vec{k}_j}$$

$$= \int d^3x\varphi_{\vec{k}_i}^*\varphi_{\vec{k}_j}\left(\frac{\hbar^2\vec{k}_j^2}{1m} + U\right), \qquad \varphi_{\vec{k}_j} = \frac{1}{\sqrt{V}}e^{i\vec{k}_j\vec{x}}$$

$$= \frac{\hbar^2\vec{k}_j^2}{2m}\delta_{k_j k_i} + \underbrace{\int d^3x\varphi_{\vec{k}_i}^* U(\vec{x})\varphi_{\vec{k}_j}}_{\frac{1}{V}U_{\vec{k}_i-\vec{k}_j}}$$

$$\Rightarrow H = \sum_{i,j}\left(\frac{\hbar^2\vec{k}_j}{2m}\delta_{\vec{k}_i\vec{k}_j}a_i^\dagger a_j + \frac{1}{V}U_{\vec{k}_i-\vec{k}_j}a_i^\dagger a_j\right)$$

$$\Rightarrow \boxed{H = \sum_{\vec{k}}\frac{\hbar^2\vec{k}^2}{2m}a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{V}\sum_{\vec{k}}\sum_{\vec{k}'}U_{\vec{k}-\vec{k}'}a_{\vec{k}}^\dagger a_{\vec{k}'}}$$

Für die Erzegungs- und Vernichtungsoperatoren zu einem bestimmten $\vec{k}$ gilt ebenfalls:

$$[a_{\vec{k}}, a_{\vec{k}'}]_\pm = 0 = [a_{\vec{k}}^\dagger, a_{\vec{k}'}^\dagger]_\pm,$$
$$[a_{\vec{k}}, a_{\vec{k}'}^\dagger]_\pm = \delta_{\vec{k}\vec{k}'}$$

Zwei-Teilchen-Wechselwirkung: $f^{(2)}(\vec{x}-\vec{x}')$
Fouriertransformierte des WW-Terms mit $\vec{y}=\vec{x}-\vec{x}'$:

$$f^{(2)}_{\vec{q}} = \int d^3y e^{-i\vec{q}\vec{y}} f^{(2)}(\vec{y})$$
$$\Rightarrow f^{(2)}(\vec{y}) = \frac{1}{V}\sum_{\vec{q}} f^{(2)}_{\vec{q}} e^{(\vec{q}-\vec{q}')\vec{y}}$$

Probe:

$$f^{(2)}_{\vec{q}} = \frac{1}{V}\int d^3y e^{-i\vec{q}\vec{y}} \sum_{\vec{q}} f^{(2)}_{\vec{q}} e^{(\vec{q}-\vec{q}')\vec{y}}$$
$$= \frac{1}{V}\sum_{\vec{q}} f^{(2)}_{\vec{q}} V\delta_{\vec{q}\vec{q}'}$$

Also ist:

$$\langle\vec{p}',\vec{k}'|f^{(2)}(\vec{x}-\vec{x}')|\vec{p},\vec{k}\rangle = \frac{1}{V^2}\int d^3\vec{x}d^3\vec{x}' e^{-i\vec{p}'\vec{x}}e^{-i\vec{k}'\vec{x}'}f^{(2)}(\vec{x}-\vec{x}')e^{i\vec{k}\vec{x}'}e^{i\vec{p}\vec{x}}$$
$$= \frac{1}{V^3}\sum_{\vec{q}} f^{(2)}_{\vec{q}} \int d^3\vec{x}d^3\vec{x}' e^{-i(\vec{p}'-\vec{p}-\vec{q})\vec{x}} e^{-i(\vec{k}'-\vec{k}+\vec{q})\vec{x}'}$$
$$= \frac{V^2}{V^3}\sum_{\vec{q}} f^{(2)}_{\vec{q}} \delta_{\vec{p}'-\vec{p}-\vec{q},0}\delta_{\vec{k}'-\vec{k}+\vec{q},0}$$
$$\Rightarrow F = \frac{1}{2}\sum_{\vec{p}\vec{p}'\vec{k}\vec{k}'} \langle\vec{p}',\vec{k}'|f^{(2)}(\vec{x}-\vec{x}')|\vec{p},\vec{k}\rangle a^\dagger_{\vec{p}'}a^\dagger_{\vec{k}'}a_{\vec{k}}a_{\vec{p}}$$
$$= \frac{1}{2V}\sum_{\vec{p}\vec{p}'\vec{k}\vec{k}'} \langle\vec{p}',\vec{k}'|f^{(2)}(\vec{x}-\vec{x}')|\vec{p},\vec{k}\rangle a^\dagger_{\vec{p}'}a^\dagger_{\vec{k}'}a_{\vec{k}}a_{\vec{p}} f^{(2)}_{\vec{q}} \delta_{\vec{p}'-\vec{p}-\vec{q},0}\delta_{\vec{k}'-\vec{k}+\vec{q},0}$$
$$\Rightarrow \boxed{F = \frac{1}{2V}\sum_{\vec{p}\vec{p}'\vec{k}\vec{k}'} \langle\vec{p}',\vec{k}'|f^{(2)}(\vec{x}-\vec{x}')|\vec{p},\vec{k}\rangle a^\dagger_{\vec{p}'}a^\dagger_{\vec{k}'}a_{\vec{k}}a_{\vec{p}} f^{(2)}_{\vec{q}}}$$

Der Dichteoperator:

$$
\begin{aligned}
\widehat{n}(\vec{x}) &= \widehat{\psi}^\dagger(\vec{x})\widehat{\psi}(\vec{x}) \\
&= \sum_{\vec{k}\vec{k}'} \varphi^*_{\vec{k}}\varphi_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} \\
&= \frac{1}{V}\sum_{\vec{k}\vec{k}'} e^{-i\vec{k}\vec{x}} e^{i\vec{k}'\vec{x}} a^\dagger_{\vec{k}} a_{\vec{k}'} \\
&\Rightarrow \widehat{n(\vec{x})} = n_{\vec{q}} = \int d^3\vec{x}\widehat{n}(\vec{x})e^{-i\vec{q}\vec{x}} \\
&= \frac{1}{V}\sum_{\vec{k}\vec{k}'} \underbrace{\int d^3\vec{x} e^{-i(\vec{k}-\vec{k}'+\vec{q})\vec{x}}}_{=V\delta_{\vec{k}-\vec{k}'+\vec{q},\vec{0}}} a^\dagger_{\vec{k}} a_{\vec{k}'} \\
&\Leftrightarrow \boxed{n_{\vec{q}} = \sum_{\vec{k}} a^{\dagger}{}_{\vec{k}-\vec{q}} a_{\vec{k}}}
\end{aligned}
$$

Bei dem Wechsel in den Impulsraum haben wir den Spinfreiheitsgrad verloren. Dieser muss nun wieder in den Formalismus aufgenommen werden:

$$
\widehat{\psi}(\vec{x}) \longrightarrow \widehat{\psi}_{s_z}(\vec{x}) \equiv \widehat{\psi}_\sigma(\vec{x}), \qquad -s \leq s_z \leq s
$$

Dann schreibt sich der Hamiltonoperator wie folgt:

$$
\begin{aligned}
H = \sum_\sigma \int d^3\vec{x} &\left(\frac{\hbar^2}{2m} \vec{\nabla}\widehat{\psi}^\dagger_\sigma(\vec{x})\vec{\nabla}\widehat{\psi}_\sigma(\vec{x}) + U(\vec{x})\widehat{\psi}^\dagger_\sigma(\vec{x})\widehat{\psi}_\sigma(\vec{x}) \right) \\
+ \frac{1}{2}\sum_\sigma\sum_{\sigma'} &\int d^3\vec{x} d^3\vec{x}' \widehat{\psi}^\dagger_\sigma(\vec{x})\widehat{\psi}^\dagger_{\sigma'}(\vec{x}') f^2(\vec{x},\vec{x}')\widehat{\psi}_{\sigma'}(\vec{x}')\widehat{\psi}_\sigma(\vec{x})
\end{aligned}
$$

Die Kommutatorrelationen ergeben sich zu:

$$
\begin{aligned}
&[\widehat{\psi}_\sigma(\vec{x}), \widehat{\psi}_{\sigma'}(\vec{x'})]_\pm = 0 = [\widehat{\psi}^\dagger_\sigma(\vec{x}), \widehat{\psi}^\dagger_{\sigma'}(\vec{x'})]_\pm, \\
&[\widehat{\psi}_\sigma(\vec{x}), \widehat{\psi}^\dagger_{\sigma'}(\vec{x}')]_\pm = \delta_{\sigma\sigma'}\delta^{(3)}(\vec{x}-\vec{x}')
\end{aligned}
$$

$$
\begin{aligned}
&\widehat{\psi}_\sigma(\vec{x}) = \sum_{\vec{k}} \varphi_{\vec{k}}(\vec{x}) a_{\vec{k},\sigma} \Rightarrow \\
&[a_{\vec{k},\sigma}, a_{\vec{k}',\sigma'}]_\pm = 0 = [a^\dagger_{\vec{k}.\sigma}, a^\dagger_{\vec{k}',\sigma'}]_\pm, \\
&[a_{\vec{k},\sigma}, a^\dagger_{\vec{k}',\sigma'}]_\pm = \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'}
\end{aligned}
$$

Aufgabe 9: Zeigen Sie folgene Relation:

$$i\hbar\frac{d}{dt}a^H_{\vec{k},\sigma} = \frac{(\hbar\vec{k})^2}{2m}a^H_{\vec{k},\sigma} + \sum_{\vec{k}'} U_{\vec{k}-\vec{k}'}a^H_{\vec{k}',\sigma} + \frac{1}{V}\sum_{\vec{p},\vec{q}}\sum_{\sigma'} f^2_{\vec{q}}a^{H\dagger}_{\vec{p}+\vec{q},\sigma'}a^H_{\vec{p},\sigma'}a^H_{\vec{k}+\vec{q},\sigma}$$

Hinweis:

$$i\hbar\frac{d}{dt}a^H_{\vec{k},\sigma} = [a^H_{\vec{k},\sigma}, H], \qquad f_{\vec{q}} = f_{-\vec{q}}$$

9 II.8 Quantisation of the electromagnatic field (version 1)

The Hamiltonian of classical electromagnetism is given by

$$H_{EM} = \frac{1}{8\pi} \int d^3x \left(|\vec{E}|^2 + |\vec{B}|^2 \right) \tag{9.1}$$

where $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields respectively. These fields obey a set of differential equations known as *Maxwell's equations*:

$$\vec{\nabla} \cdot \vec{B} = 0 \qquad \vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 \tag{9.2}$$

$$\vec{\nabla} \cdot \vec{E} = \rho \qquad \vec{\nabla} \times \vec{B} - \frac{1}{c}\frac{\partial \vec{E}}{\partial t} = \vec{j} \tag{9.3}$$

Equations (9.2) are the homogeneous and (9.3) the inhomogeneous Maxwell's equations which contain source terms, namely a charge desity ρ and a current density $\vec{j}$. The homogeneous equations are solved by introducing a vector potential $\vec{A}$ and a scalar potential ϕ satisfying

$$\vec{B} = \vec{\nabla} \times \vec{A} \tag{9.4}$$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \vec{\nabla}\phi \, . \tag{9.5}$$

When it comes to quantising electromagnetism it is not the $\vec{E}$ und $\vec{B}$ fields that we will try to quantise, but the potentials $(\phi, \vec{A})$. Classically, ϕ and $\vec{A}$ only serve as auxillary fields which simplify many equations that would be much harder to solve purely in terms of $\vec{E}$ and $\vec{B}$, but in quantum mechanics these two potentials play a much more fundamental role. If we couple elctromagnetism to matter, for instance, the Hamiltonian will pick up an extra piece

$$H_{matter} = \sum_\alpha \left[\frac{1}{2m_\alpha} \left(\vec{p}_\alpha - \frac{e}{c}\vec{A}(\vec{x}_\alpha) \right)^2 + e\phi(\vec{x}_\alpha) + V(\vec{x}_\alpha) \right] \tag{9.6}$$

involving ϕ and $\vec{A}$ rather than the observable electric or magnetic fields.
But before we move on, we note that ϕ and $\vec{A}$ are not uniquely determined by equations (9.4) and (9.5), because if we move the fields by

$$\vec{A} \longrightarrow \vec{A}' = \vec{A} + \vec{\nabla}\Lambda \tag{9.7}$$

$$\phi \longrightarrow \phi' = \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t} \tag{9.8}$$

where $\Lambda = \Lambda(\vec{x}, t)$ is an arbitrary smooth function of space and time, this will leave the physical fields $\vec{E}$ and $\vec{B}$ invariant. This fact is known as *gauge invariance* and means that $(\phi, \vec{A})$ contains unphysical degrees of freedom which we have to devide out before we quantise the theory. When quantised, excitations of each degree of freedom will appear as particles, so we need to be very careful to only consider those degrees of freedom that are actually physical in order to get the right particle excitations out of our quantisation procedure.
In this particular case we can fix the gauge (and thus eliminate unphysical information) by imposing the Coulomb gauge condition

$$\vec{\nabla} \cdot \vec{A} = 0\,. \tag{9.9}$$

Also we will only quantise the free fields (ρ and $\vec{j}$ are being set to zero) and hence the first inhomogeneous Maxwell equation now reads

$$0 = \vec{\nabla} \cdot \vec{E} = \vec{\nabla} \cdot (-\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \vec{\nabla}\phi) = -\triangle\phi \tag{9.10}$$

where we have used the Coulomb gauge condition to come to the last expression. This means ϕ is a harmonic function solving the *Laplace equation* $\triangle\phi = 0$. Solutions to this equation are well known and can be expressed in terms of the Bessel functions P_ℓ

$$\phi = \sum_{\ell=0}^{\infty} \left(a_\ell r^\ell + b_\ell r^{-(\ell+1)}\right)\ P_\ell(\cos\theta) \tag{9.11}$$

where r and θ are the radial and azimuthal coordinate in spherical polar coordinates. We demand that ϕ be regular at $r = 0$ and at $r \to \infty$ which gives $b_\ell = 0$ and $a_\ell = 0$ respectively. Thus, we must have

$$\phi = 0 \quad . \tag{9.12}$$

The only remaining Maxwell equation is now $\vec{\nabla} \times \vec{B} - \frac{1}{c}\frac{\partial \vec{E}}{\partial t} = 0$. Plugging in (9.5) and (9.12) yields

$$0 = \vec{\nabla} \times \vec{\nabla} \times \vec{A} - \frac{1}{c}\frac{\partial}{\partial t}\left(-\frac{1}{c}\frac{\partial \vec{A}}{\partial t}\right) = -\left(\triangle - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{A} \tag{9.13}$$

using the identity $\vec{\nabla} \times \vec{\nabla} \times \vec{A} = -\triangle\vec{A} + \vec{\nabla}(\vec{\nabla} \cdot \vec{A})$ and the Coulomb gauge $\vec{\nabla} \cdot \vec{A} = 0$. The differential operator $\Box \equiv (\triangle - \frac{1}{c^2}\frac{\partial^2}{\partial t^2})$ is known as the *d'Alembert operator* or *wave operator*. The equation we are left with can simply be rewritten as

$$\Box\vec{A} = 0 \quad . \tag{9.14}$$

Solutions to (9.14) are given by

$$\vec{A} = \sum_{\vec{k}} \mathrm{Re}\left(\vec{A}_{\vec{k}}\, e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}\right) \tag{9.15}$$

with $\omega_{\vec{k}} = c|\vec{k}|$ and some constant amplitudes $\vec{A}_{\vec{k}}$. The reason why there is a discrete sum over values of $\vec{k}$ (which we have left unspecified) is that we once again imagine putting the whole system in a box of a finite volume V such that only a discrete set of momenta is allowed. To show that (9.15) is a solution we simply evaluate

$$\begin{aligned}
\Box\vec{A} &= \sum_{\vec{k}} \mathrm{Re}\left(\vec{A}_{\vec{k}}\, \Box\, e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}\right) \\
&= \sum_{\vec{k}} \mathrm{Re}\left(\vec{A}_{\vec{k}} \left(\triangle - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}\right) \\
&= \sum_{\vec{k}} \mathrm{Re}\left(\vec{A}_{\vec{k}} \left(-\vec{k}^2 + \frac{1}{c^2}\omega_{\vec{k}}^2\right) e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}\right) \\
&= 0
\end{aligned}$$

since the inner bracket vanishes.

The result (9.15) was derived in the Coulomb gauge, so we have to demand

$$0 = \vec{\nabla}\cdot\vec{A} = \sum_{\vec{k}} i\vec{k}\cdot\vec{A}_{\vec{k}}\, e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)} \tag{9.16}$$

$$\Longrightarrow \qquad \vec{k}\cdot\vec{A}_{\vec{k}} = 0 \quad \forall\vec{k} \quad . \tag{9.17}$$

Thus, we found that for all values of $\vec{k}$ the amplitudes $\vec{A}_{\vec{k}}$ must be orthogonal to $\vec{k}$ which points in the direction of propagation of the plane wave solution $e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}$. It also says that there are only *two independent degrees of freedom* left in $\vec{A}_{\vec{k}}$, although we started out with four independent fields $(\phi, \vec{A})$. The gauge condition removed two degrees of freedom which is exactly what one would expect as the photon (which will be the particle that comes out of the quantisation of Maxwell's theory) has precisely these two degrees of freedom, i.e. the two possible spin polarisations. To make this more clear we will rewrite $\vec{A}_{\vec{k}}$ in a slightly more suggestive way

$$\vec{A}_{\vec{k}} = \mathcal{N}\sum_{\lambda=1}^{2} \vec{\varepsilon}_{\vec{k},\lambda}\, a_{\vec{k},\lambda} \tag{9.18}$$

where $a_{\vec{k},\lambda}$ are just numbers, $\mathcal{N}$ is an additional normalisation to be specified later, and $\{\vec{\varepsilon}_{\vec{k},1}\,,\,\vec{\varepsilon}_{\vec{k},2}\}$ is an orthonormal basis of the subspace orthogonal to $\vec{A}_{\vec{k}}$ for each $\vec{k}$, i.e.

$$\vec{k}\cdot\vec{\varepsilon}_{\vec{k},\lambda}=0 \quad \text{and} \quad \vec{\varepsilon}_{\vec{k},\lambda}\cdot\vec{\varepsilon}_{\vec{k},\lambda'}=\delta_{\lambda\lambda'} \quad . \tag{9.19}$$

We can also choose $\vec{\varepsilon}_{\vec{k},\lambda}$ to satisfy

$$\begin{aligned}\vec{k}\times\vec{\varepsilon}_{\vec{k},1} &= \vec{\varepsilon}_{\vec{k},2}\,|\vec{k}| && (9.20)\\ \vec{k}\times\vec{\varepsilon}_{\vec{k},2} &= -\vec{\varepsilon}_{\vec{k},1}\,|\vec{k}| \quad . && (9.21)\end{aligned}$$

Having that in hand we can now compute the explicit form of the $\vec{E}$ and $\vec{B}$ fields which solve the free Maxwell equations

$$\vec{B}=\vec{\nabla}\times\vec{A}=\sum_{\vec{k}}\sum_{\lambda} i\vec{k}\times\vec{\varepsilon}_{\vec{k},\lambda}\mathcal{N}\,\mathcal{A}(\vec{k},\lambda) \tag{9.22}$$

and

$$\vec{E}=-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}=\sum_{\vec{k}}\sum_{\lambda} i\frac{\omega_{\vec{k}}}{c}\,\vec{\varepsilon}_{\vec{k},\lambda}\mathcal{N}\,\mathcal{A}(\vec{k},\lambda) \tag{9.23}$$

where $\mathcal{A}(\vec{k},\lambda)$ stands for

$$\mathcal{A}(\vec{k},\lambda)=\left(a_{\vec{k},\lambda}\,e^{i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}-a^{\dagger}_{\vec{k},\lambda}\,e^{-i(\vec{k}\vec{x}-\omega_{\vec{k}}t)}\right) \ . \tag{9.24}$$

(For later convenience we have already written $a^{\dagger}_{\vec{k},\lambda}$ for the complex conjugation of $a_{\vec{k},\lambda}$.) The main goal of this chapter is to write the Hamiltonian

$$H=\frac{1}{8\pi}\int d^3x\,\left(|\vec{E}|^2+|\vec{B}|^2\right) \tag{9.25}$$

in terms of $a_{\vec{k},\lambda}$ and $a^{\dagger}_{\vec{k},\lambda}$. This expression will involve factors of the form $I:=\int d^3x\mathcal{A}(\vec{k},\lambda)\,\mathcal{A}(\vec{k}',\lambda')$ which we will compute first. What we get is

$$\begin{aligned} I &= \int d^3x\,\mathcal{A}(\vec{k},\lambda)\,\mathcal{A}(\vec{k}',\lambda')\\ &= \int d^3x\,\Big(a_{\vec{k},\lambda}\,a_{\vec{k}',\lambda'}\,e^{i(\vec{k}+\vec{k}')\vec{x}}\,e^{-i(\omega_{\vec{k}}+\omega_{\vec{k}'})t}+a^{\dagger}_{\vec{k},\lambda}\,a^{\dagger}_{\vec{k}',\lambda'}\,e^{-i(\vec{k}+\vec{k}')\vec{x}}\,e^{i(\omega_{\vec{k}}+\omega_{\vec{k}'})t}\\ &\qquad -a_{\vec{k},\lambda}\,a^{\dagger}_{\vec{k}',\lambda'}\,e^{i(\vec{k}-\vec{k}')\vec{x}}\,e^{-i(\omega_{\vec{k}}-\omega_{\vec{k}'})t}-a^{\dagger}_{\vec{k},\lambda}\,a_{\vec{k}',\lambda'}\,e^{-i(\vec{k}-\vec{k}')\vec{x}}\,e^{i(\omega_{\vec{k}}-\omega_{\vec{k}'})t}\Big) \ . \end{aligned}$$

We use the identity

$$\int d^3x\, e^{i(\vec{k}-\vec{k}')\vec{x}} = V\,\delta_{\vec{k}\vec{k}'} \tag{9.26}$$

on this integral and get

$$\begin{aligned} I &= V\Big[\delta_{\vec{k},-\vec{k}'}\left(a_{\vec{k},\lambda}\,a_{-\vec{k},\lambda'}\,e^{-2i\omega_{\vec{k}}t} + a^\dagger_{\vec{k},\lambda}\,a^\dagger_{-\vec{k},\lambda'}\,e^{2i\omega_{\vec{k}}t}\right) \\ &\quad -\delta_{\vec{k}\vec{k}'}\left(a_{\vec{k},\lambda}\,a^\dagger_{\vec{k},\lambda'} + a^\dagger_{\vec{k},\lambda}\,a_{\vec{k},\lambda'}\right)\Big]\,. \end{aligned}$$

The Hamiltonian can now be written as

$$\begin{aligned} H &= \frac{1}{8\pi}\int d^3x\,\Bigg(\sum_{\vec{k},\lambda}\sum_{\vec{k}',\lambda'}\mathcal{N}^2\,\frac{\omega_{\vec{k}}\omega_{\vec{k}'}}{c^2}\,\vec{\varepsilon}_{\vec{k},\lambda}\cdot\vec{\varepsilon}_{\vec{k}',\lambda'}\,\mathcal{A}(\vec{k},\lambda)\,\mathcal{A}(\vec{k}',\lambda') \\ &\qquad + \sum_{\vec{k},\lambda}\sum_{\vec{k}',\lambda'}\mathcal{N}^2\,(\vec{k}\times\vec{\varepsilon}_{\vec{k},\lambda})\cdot(\vec{k}'\times\vec{\varepsilon}_{\vec{k}',\lambda'})\,\mathcal{A}(\vec{k},\lambda)\,\mathcal{A}(\vec{k}',\lambda')\Bigg) \\ &= \frac{1}{8\pi}\sum_{\vec{k},\lambda}\sum_{\vec{k}',\lambda'}\mathcal{N}^2\left(\frac{\omega_{\vec{k}}\omega_{\vec{k}'}}{c^2}\vec{\varepsilon}_{\vec{k},\lambda}\cdot\vec{\varepsilon}_{\vec{k}',\lambda'} + (\vec{k}\times\vec{\varepsilon}_{\vec{k},\lambda})\cdot(\vec{k}'\times\vec{\varepsilon}_{\vec{k}',\lambda'})\right) I \\ &= \sum_{\vec{k}}\sum_{\lambda\lambda'}\frac{V\mathcal{N}^2}{8\pi}\Bigg[\left(\frac{\omega^2_{\vec{k}}}{c^2}\,\vec{\varepsilon}_{\vec{k},\lambda}\cdot\vec{\varepsilon}_{-\vec{k},\lambda'} - |\vec{k}|^2\delta_{\lambda\lambda'}\right)\left(a_{\vec{k},\lambda}\,a_{-\vec{k},\lambda'}\,e^{-2i\omega_{\vec{k}}t} + a^\dagger_{\vec{k},\lambda}\,a^\dagger_{-\vec{k},\lambda'}\,e^{2i\omega_{\vec{k}}t}\right) \\ &\qquad + \left(\frac{\omega^2_{\vec{k}}}{c^2}\,\vec{\varepsilon}_{\vec{k},\lambda}\cdot\vec{\varepsilon}_{-\vec{k},\lambda'} + |\vec{k}|^2\delta_{\lambda\lambda'}\right)\left(a_{\vec{k},\lambda}\,a^\dagger_{\vec{k},\lambda'} + a^\dagger_{\vec{k},\lambda}\,a_{\vec{k},\lambda'}\right)\Bigg] \\ &= \sum_{\vec{k}}\sum_{\lambda\lambda'}\frac{V|\vec{k}|^2\mathcal{N}^2}{8\pi}\Big[(\delta_{\lambda\lambda'}-\delta_{\lambda\lambda'})\left(a_{\vec{k},\lambda}\,a_{-\vec{k},\lambda'}\,e^{-2i\omega_{\vec{k}}t} + a^\dagger_{\vec{k},\lambda}\,a^\dagger_{-\vec{k},\lambda'}\,e^{2i\omega_{\vec{k}}t}\right) \\ &\qquad +2\delta_{\lambda\lambda'}\left(a_{\vec{k},\lambda}\,a^\dagger_{\vec{k},\lambda'} + a^\dagger_{\vec{k},\lambda}\,a_{\vec{k},\lambda'}\right)\Big] \\ &= \sum_{\vec{k},\lambda}\frac{V|\vec{k}|^2\mathcal{N}^2}{4\pi}\left(a_{\vec{k},\lambda}\,a^\dagger_{\vec{k},\lambda} + a^\dagger_{\vec{k},\lambda}\,a_{\vec{k},\lambda}\right)\,. \end{aligned}$$

Now we can choose a nice normalisation and set $\mathcal{N}^2 = \frac{2\pi\hbar c}{V|\vec{k}|}$. With this convention the Hamiltonian takes the form

$$\boxed{H = \sum_{\vec{k},\lambda}\frac{\hbar\omega_{\vec{k}}}{2}\left(a_{\vec{k},\lambda}\,a^\dagger_{\vec{k},\lambda} + a^\dagger_{\vec{k},\lambda}\,a_{\vec{k},\lambda}\right)} \tag{9.27}$$

which we immediately recognise as the Hamiltonian of a system of infinitely many uncoupled harmonic oscillators.

From equation (9.27) the quantisation of Maxwell's theory is straightforward. We simply promote $a_{\vec{k},\lambda}$ and $a^\dagger_{\vec{k},\lambda}$ to operators acting on a Fock space $\mathcal{H}$ such that they satisfy the canonical commutation relations

$$[a_{\vec{k},\lambda}\,,\,a_{\vec{k}',\lambda'}] = [a^\dagger_{\vec{k},\lambda}\,,\,a^\dagger_{\vec{k}',\lambda'}] = 0 \tag{9.28}$$

$$[a_{\vec{k},\lambda}\,,\,a^\dagger_{\vec{k}',\lambda'}] = \delta_{\vec{k}\vec{k}'}\,\delta_{\lambda\lambda'}\,. \tag{9.29}$$

We define the vacuum state $|0\rangle \in \mathcal{H}$ as the state that is annihilated by all annihilation operators

$$a_{\vec{k},\lambda}\,|0\rangle = 0 \quad \forall \vec{k},\lambda \tag{9.30}$$

and then one- and two-particle states are given by

$$|\vec{k},\lambda\rangle = a^\dagger_{\vec{k},\lambda}\,|0\rangle \tag{9.31}$$

$$|\vec{k}_1,\lambda_1;\vec{k}_2,\lambda_2\rangle = a^\dagger_{\vec{k}_2,\lambda_2}a^\dagger_{\vec{k}_1,\lambda_1}\,|0\rangle \tag{9.32}$$

respectively. The one-particle state $|\vec{k},\lambda\rangle$ is usually called a *photon* with momentum $\vec{k}$ and polarisation λ.

In the next section we will look at the emission of such a photon by an atom in an excited state. To that end we need one additional formula which we will now quickly derive. In equation (9.6) we had the interaction Hamiltonian with matter as

$$H_{matter} = \sum_\alpha \left[\frac{1}{2m}\left(\vec{p}_\alpha - \frac{e}{c}\vec{A}(\vec{x}_\alpha)\right)^2 + e\phi(\vec{x}_\alpha) + V(\vec{x}_\alpha)\right]\,.$$

This Hamiltonian can be split into two pieces $H = H_0 + H_1$ where

$$H_0 = \sum_\alpha \left(\frac{1}{2m}\vec{p}^{\,2}_\alpha + V(\vec{x}_\alpha)\right) \tag{9.33}$$

and

$$H_1 = \sum_\alpha \left(-\frac{e}{2mc}(\vec{p}_\alpha\vec{A} + \vec{A}\vec{p}_\alpha) + \frac{e^2}{2mc^2}\vec{A}^2 + e\phi\right)\,. \tag{9.34}$$

It is easy to check that if you set

$$\rho(\vec{x}) = \sum_\alpha \delta(\vec{x}-\vec{x}_\alpha) \quad \text{and} \quad \vec{j}(\vec{x}) = \frac{1}{2m}\sum_\alpha \left[\vec{p}_\alpha\delta(\vec{x}-x_\alpha) + \delta(\vec{x}-x_\alpha)\vec{p}_\alpha\right]$$

H_1 becomes

$$H_1 = \int d^3x \left(-\frac{e}{c}\,\vec{j}(\vec{x})\cdot\vec{A}(\vec{x}) + \frac{e^2}{2mc^2}\,\rho(\vec{x}) + e\,\rho(\vec{x})\phi(\vec{x})\right)\,. \tag{9.35}$$

That is the equation we were after and which will be of some use in the next section.

10 Emission of photons - time-dependant pertubation theory

$$
\begin{aligned}
H &= H_0 + V(t) \\
H_0|n\rangle &= E_0|n\rangle
\end{aligned}
$$

Interaction-picture:

$$
\left.\begin{array}{l}
|\psi\rangle_I = e^{\frac{iH_0 t}{\hbar}}|\psi\rangle \\
V_I = e^{\frac{iH_0 t}{\hbar}} V e^{\frac{iH_0 t}{\hbar}}
\end{array}\right\} \longrightarrow \boxed{i\hbar\frac{\partial}{\partial t}|\psi\rangle_I = \cdots = V_I|\psi\rangle_I}
$$

$$
\begin{aligned}
|\psi(t)\rangle_I &= |\psi(t_0)\rangle_I + \frac{1}{i\hbar}\int_{t_0}^{t} \mathrm{dt}'\ V_i(t')|\psi(t')\rangle_I \\
&= \underbrace{|\psi(t_0)\rangle_I}_{|m\rangle-\text{Eigenstate of } H_0} + \frac{1}{i\hbar}\int_{t_0}^{t} \mathrm{dt}'\ V_i(t')|\psi(t_0)\rangle_I + \underbrace{O(V_I^2)}_{\text{unimportant for "small" V}}
\end{aligned}
$$

transition amplitude for $|m\rangle \rightarrow |n\rangle$:

$$
\begin{aligned}
\langle n(t)|\psi(t)\rangle &= \langle n|\underbrace{e^{\frac{iH_0 t}{\hbar}}|\psi(t)\rangle}_{|\psi\rangle_I} \\
&= \langle n|\psi\rangle_I \\
&= \underbrace{\langle n|m\rangle}_{\delta_{nm}} + \frac{1}{i\hbar}\int_{t_0}^{t} \mathrm{dt}'\ \langle n|V_I(t')|m\rangle \\
&= \delta_{nm} + \frac{1}{i\hbar}\int_{t_0}^{t} \mathrm{dt}'\ e^{\frac{i(E_n^0 - E_m^0)}{\hbar}t'}\langle n|V(t')|m\rangle
\end{aligned}
$$

From quantum mechanics I:

$$
\begin{aligned}
V(t') &= \theta(t')V \\
P_{\substack{m\rightarrow n \\ m\neq n}} &= |\langle n(t)|\psi(t)\rangle|^2 \\
= \dots &= \frac{1}{\hbar}\left(\frac{\sin\left(\frac{\omega_{mn}t}{2}\right)}{\frac{\omega_{mn}t}{2}}\right)^2 |\langle n|V|m\rangle|^2 \\
&\quad \left(\text{with } \omega_{mn} = \frac{1}{\hbar}\left(E_n^0 - E_m^0\right)\right)
\end{aligned}
$$

$$\boxed{\Gamma_{mn} \lim_{t\to\infty} \frac{1}{t} P_{m\to n} = \frac{2\pi}{\hbar\delta(E_n^0 - E_m^0)|\langle n|V|m\rangle|^2}}$$

Fermi's golden rule

now(in quantum mechanics II): periodic pertubation

$$\begin{aligned} V(t) &= \Theta(t)\left(Fe^{-i\omega t} + F^\dagger e^{i\omega t}\right) \\ \hookrightarrow \langle n(t)|\psi(t)\rangle &= \frac{1}{\hbar}\int_0^t \mathrm{d}t' \left[e^{i(\omega_{mn}-\omega)t'}\langle n|F|m\rangle + e^{i(\omega_{mn}+\omega)t'}\langle n|F^\dagger|m\rangle\right] \\ &= \dots \end{aligned}$$

$$\boxed{\Gamma_{mn} = \frac{2\pi}{\hbar}\left[\delta(E_n^0 - E_m^0 - \hbar\omega)|\langle n|F|m\rangle|^2 + \delta(E_n^0 - E_m^0 + \hbar\omega)|\langle n|F^\dagger|m\rangle|^2\right]}$$

Application: initial state of H: Electon in $|m\rangle$ no photon $|0\rangle$
final state of H: $|n\rangle$ photon $a^\dagger_{\vec{k}\lambda}|0\rangle$

$$V = H_1 \overset{\phi=0}{=} \int \mathrm{d}^3\mathrm{x}\left(-\frac{e}{c}\vec{j}\vec{A} + \frac{e^2}{2mc}\underbrace{\rho\vec{A}^2}_{\substack{\text{cannot contribute}\\(\vec{A}^2\propto a^{\dagger 2}_{\vec{k}\lambda})}}\right)$$

$$\hookrightarrow \Gamma_{mn} = \frac{2\pi}{\hbar}\frac{e^2}{c^2}\delta(E_m - E_n - \hbar c\vec{k})\left|\langle n|\langle 0|a_{\vec{k}\lambda}\int \mathrm{d}^3\mathrm{x}\,\vec{j}\vec{A}\,|0\rangle|m\rangle\right|^2$$

10.1 Spontaneous Emission of photons

$$\left.\begin{array}{llll} \text{Initial state} & |m\rangle & |0\rangle & \\ & \uparrow & \uparrow & \\ & e^- & \gamma & \leftarrow \text{Photon} \\ & \downarrow & \downarrow & \\ \text{Final state} & |n\rangle & a^\dagger_{\vec{k},\ \lambda}|0\rangle & \end{array}\right\}\text{compute with Fermi' s golden rule}$$

$$\Gamma_{m\to n,\vec{k},\lambda} = \frac{2\pi}{\hbar}\frac{e^2}{c^2}\,\delta(E_m - E_n - \hbar c|\vec{k}|)\;|\ldots|^2$$

$$|\ldots|^2 = \underbrace{|\langle n|\langle 0|a_{\vec{k},\lambda}}_{\text{final state}}\left(\int \mathrm{d}^3\mathrm{x}\;\vec{j}\sum_{\vec{k}',\lambda'}\vec{\epsilon}_{\vec{k}',\lambda'}\left(a_{\vec{k}'\lambda'}e^{i\vec{k}'\vec{x}} + a^\dagger_{\vec{k}\lambda}e^{-i\vec{k}\vec{x}}\right)\right)\underbrace{|0\rangle|m\rangle}_{\text{initial state}}\;|^2$$

$$V = \int \mathrm{d}^3\mathrm{x}\left(-\frac{e}{c}\vec{j}\vec{A} + \frac{e^2}{2mc}\rho\vec{A}^2\right)$$

$$|\ldots|^2 = |\langle n|\int \mathrm{d}^3\mathrm{x}\;\vec{j}\;\vec{\epsilon}_{\vec{k},\lambda}e^{-i\vec{k}\vec{x}}|m\rangle|^2$$

$$\vec{j}\vec{k} \equiv \int \mathrm{d}^3\mathrm{x}\;\vec{j}(\vec{x})e^{-i\vec{k}\vec{x}}$$

$$\underset{\substack{\uparrow\\ \text{visible}\\ \text{light}}}{\simeq} \int \mathrm{d}^3\mathrm{x}\;\vec{j}(\vec{x})\Big(\underset{\substack{\uparrow\\ \text{electric}\\ \text{dipol}\\ \text{transition}}}{1} - \underset{\substack{\uparrow\\ \text{magnetic}\\ \text{dipol}\\ \text{transition}}}{i\vec{k}\vec{x}} - \underset{\substack{\uparrow\\ \text{electric}\\ \text{quadrupol}\\ \text{transition}}}{\frac{1}{2}(\vec{k}\vec{x})^2} + \ldots\Big)$$

$$\Rightarrow |\ldots|^2 \underset{\substack{\uparrow\\ \text{electric}\\ \text{dipol}\\ \text{transition}}}{=} |\langle n|\vec{j}_0\vec{\epsilon}_{0\lambda}|m\rangle|^2$$

$$\vec{j}_0 = \int \mathrm{d}^3\mathrm{x}\;\vec{j}(\vec{x}) \underset{\substack{\uparrow\\ \text{last}\\ \text{lecture}}}{=} \frac{1}{2m}\int \mathrm{d}^3\mathrm{x}\sum_\alpha\left(\vec{P}_\alpha\delta(\vec{x}-\vec{x}_\alpha) + \delta(\vec{x}-\vec{x}_\alpha)\vec{P}_\alpha\right)$$

$$\int \mathrm{dx}\,\delta'(x)f(x) = f'(0) \longrightarrow = \frac{1}{m}\sum_\alpha\vec{P}_\alpha = \frac{1}{m}\underline{\vec{P}}\;;\;\underline{\vec{P}} = \sum_\alpha\vec{P}_\alpha \text{ center of mass momentum}$$

$$\vec{j}_0 = \frac{1}{m}\underline{\vec{P}} = \frac{i}{\hbar}[H_0,\underline{\vec{X}}]\;;\;\underline{\vec{X}} = \sum_\alpha\vec{x}_\alpha$$

$$\langle n|\vec{j}_0|m\rangle = \frac{i}{\hbar}(E_n - E_m)\langle n|\underline{\vec{X}}|m\rangle$$

selection rules:

$$[L_i, x_j] = i\hbar\sum_{k=1}^{3}\varepsilon_{ijk}x_k \Rightarrow [L_z, z] = 0$$

$$[L_z, x \pm iy] = \pm\hbar(x \pm iy)$$

$$|n\rangle = |n,l',m'\rangle \qquad 0 = \langle l'm'|[L_z,z]|lm\rangle = \hbar(m'-m)\langle l'm'|z|lm\rangle \Rightarrow \boxed{m'=m}$$

$$|m\rangle = |m,l,m\rangle \qquad 0 = \langle l'm'|[L_z,x\pm iy]|lm\rangle = \hbar(m'-m)\langle l'm'|x\pm iy|lm\rangle \pm \hbar\langle l'm'|x\pm iy|lm\rangle$$

$$\Leftrightarrow 0 = \hbar(m'-m\mp 1)\langle l'm'|x\pm iy|lm\rangle \Rightarrow \boxed{m'=m\pm 1}$$

selection rules for l: little known fact: $[\vec{L}^2,[\vec{L}^2,\vec{x}]] = 2\hbar\{\vec{x},\vec{L}^2\}$

$$\begin{aligned}
\langle l'm'|[\vec{L}^2,[\vec{L}^2,\vec{x}]]|lm\rangle &= -\hbar(l(l+1)-(l'(l'+1))\langle l'm'|[\vec{L}^2,\vec{x}]|lm\rangle \\
&= \hbar^4(l(l+1))-l'(l'+1))^2\langle l'm'|\vec{x}|lm\rangle \\
&= 2\hbar^2\langle l'm'|\{\vec{x},\vec{L}^2\}|lm\rangle \\
&= 2\hbar^4(l(l+1))+l'(l'))\langle l'm'|\vec{x}|lm\rangle \\
0 &= \langle l'm'|\vec{x}|lm\rangle[(l(l+1)-l'(l'+1))^2-2(l(l+1)+l'(l'+1))] \\
&= \langle l'm'|\vec{x}|lm\rangle(l+l')(l+l'+2)[(l-l')^2-1]
\end{aligned}$$

$$\Rightarrow \boxed{\begin{array}{l|l} l=l'=0 & m'=m \\ l'=l\pm 1 & m'=m\pm 1 \end{array}}$$

11 Relativistic wave-equation

11.1 Special Relativity

By: Sebastian Jakobs

Newton's Laws revisited:

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = m\ddot{\mathbf{x}} \tag{11.1}$$

$$\leftrightarrow \quad F_i = m\ddot{x}_i \tag{11.2}$$

These laws are invariant under Galilei-Transformations

$$\mathbf{x} \rightarrow \mathbf{x}' = \mathbf{x} + \mathbf{v}t + \mathbf{a} \tag{11.3}$$

$$t \rightarrow t' = t + t_0 \tag{11.4}$$

where $\mathbf{v}$ and $\mathbf{a}$ are constant vectors and t_0 is a constant time. The Newton-equations are also **covariant** (i.e. equivariant) under rotations:

$$x^i \rightarrow x'^i = \sum_k D^i_k x^k \tag{11.5}$$

Rotations change only the direction of a vector, the length is constant under rotations. Therfore

$$\sum_i x'^i x'^i = \sum_{i,k,l} D^i_k x^k D^i_l x^l \tag{11.6}$$

$$= \sum_j x^j x^j \tag{11.7}$$

$$\rightarrow \quad \sum_i D^i_k D^i_l = \delta_{kl} \tag{11.8}$$

$$\rightarrow \quad D^T D = \mathbf{1} \tag{11.9}$$

(11.8) are 6 independent equations, hence D depends on 9-6=3 independent parameters. The Matrices D are elements of the Group O(3). But since the Rotation-matrices must continuously connected with the identity $\det D = +1$ and therfore $D \in SO(3)$, where SO(3) is a Lie-Group.

In the rotated coordinate system the Newton-equations read as:

$$F'^i = m\ddot{x}'^i \tag{11.10}$$

$$\sum_k D^i_k F^k = m \sum_k D^i_k \ddot{x}'^k \tag{11.11}$$

$$\rightarrow \quad \sum_k D^i_k \left(F^k - m\ddot{x}^k\right) = 0 \tag{11.12}$$

Hence the Newton-equations are also variant under rotations.

The Galilei-principle The Physics in coordinate systems (CS) related by Galilei-transformation (incl. Rotations) is identical.
The problem which arises here is: The Maxwell-equations are not invariant/covariant under Galilei-transformations. c=const (c: Speed of light) which was shown in the experiments by Michelson and Moreley.
Einstein therefore looked for symetries of the Maxwell-equations.

Einstein-principle Physics is identical in all CS which are related by transformations that leave c=const.
For the curve of a light ray this means

$$\begin{aligned} const = c^2 &= \frac{d\mathbf{x}}{dt} \cdot \frac{d\mathbf{x}}{dt} && (11.13)\\ &= \frac{d\mathbf{x}'}{dt} \cdot \frac{d\mathbf{x}'}{dt} && (11.14)\\ &\leftrightarrow (ct)^2 - \mathbf{x}^2 = (ct')^2 - \mathbf{x}'^2 && (11.15) \end{aligned}$$

$$ds^2 = c^2 dt^2 - (d\mathbf{x})^2 = \text{const in all CS} \tag{11.16}$$

ds is the line-element.

Definition 3. *A **4-vector** is a space-time point*

$$x^\mu = (x^0, x^1, x^2, x^3) \tag{11.17}$$

where $x^0 = ct$

The line-element then is

$$ds^2 = (dx^0)^2 - (d\mathbf{x})^2 = \sum_{\mu=0}^{3} \sum_{\nu=0}^{3} \eta_{\mu\nu} dx^\mu dx^\nu \tag{11.18}$$

and

$$\eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

The x^μ are coordinates of Minkowskispace M_4 and $\eta_{\mu\nu}$ is the metric of M_4 (pseudo-euclidian-metric).

Definition 4. *A* ***contravariant 4-vector*** *is*

$$a^\mu = (a^0, \boldsymbol{a}) \tag{11.19}$$

A ***contravariant 4-vector*** *is*

$$\begin{aligned} a_\mu &= \sum_\nu \eta_{\mu\nu} a^\nu & (11.20) \\ &= (a^0, -\boldsymbol{a}) & (11.21) \end{aligned}$$

Definition 5. *The* ***scalar product*** *of 4-vectors is*

$$\begin{aligned} \langle a^\mu | b^\nu \rangle &= \sum_\mu a^\mu b_\mu = \sum_{\mu,\nu} \eta_{\mu\nu} a^\mu b^\nu & (11.22) \\ &= a^0 b^0 - \boldsymbol{a} \cdot \boldsymbol{b} & (11.23) \end{aligned}$$

Which transformations leave the scalar product invariant, which are the rotations in M_4?

Definition 6. *The* ***Lorentztransformations*** *are the coordinate transformations in* M_4

$$x^\mu \rightarrow x'^\mu = \sum_\nu \Lambda^\mu{}_\nu x^\nu \tag{11.24}$$

such that

$$\sum_\mu x'^\mu x'_\mu = \sum_\mu x^\mu x_\mu \tag{11.25}$$

From this we can conclude

$$\begin{aligned} \sum_{\mu,\nu} \eta_{\mu\nu} x'^\mu x'^\nu &= \sum_{mu,\nu} \sum_{\rho,\sigma} \eta_{\mu\nu} \Lambda^\mu{}_\rho \Lambda^\nu{}_\sigma x^\rho x^\sigma & (11.26) \\ &= \sum_{\rho,\sigma} \eta_{\rho\sigma} x^\rho x^\sigma & (11.27) \\ &\rightarrow \sum_{\mu,\nu} \eta_{\mu\nu} \Lambda^\mu{}_\rho \Lambda^\nu{}_\sigma = \eta_{\rho\sigma} & (11.28) \end{aligned}$$

$$\Lambda^T \eta \Lambda = \eta \tag{11.29}$$

One kind of solutions to this equation are the rotations

$$\Lambda = \begin{pmatrix} 1 & 0 \\ 0 & D \end{pmatrix}$$

Count the parameters of Λ: $6 = \underbrace{3}_{\text{rotation angles}} + \underbrace{3}_{\text{boost directions}}$.

The corresponding group is the orthogonal group O(1,3), where the numbers indicates the signature of the underlying metric (1 plus, 3 minuses).

Lorentz boost Consider the simplified Lorentz boost $\mathbf{v} = v\mathbf{e}_x$. The Lorentztransformation now reads as:

$$\Lambda = \begin{pmatrix} \Lambda^0{}_0 & \Lambda^0{}_1 & 0 & 0 \\ \Lambda^1{}_0 & \Lambda^1{}_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} (ct') &= \Lambda^0{}_0 ct + \Lambda^0{}_1 x && (11.30) \\ x' &= \Lambda^1{}_0 ct + \Lambda^1{}_1 x && (11.31) \\ y' &= y && (11.32) \\ z' &= z && (11.33) \end{aligned}$$

If we consider (11.25) we get the following equations:

$$\begin{aligned} (\Lambda^0{}_0)^2 - (\Lambda^1{}_0)^2 &= 1 && (11.34) \\ (\Lambda^0{}_1)^2 - (\Lambda^1{}_1)^2 &= -1 && (11.35) \\ \Lambda^0{}_0\Lambda^0{}_1 - \Lambda^1{}_0\Lambda^1{}_1 &= 0 && (11.36) \end{aligned}$$

The solutions to these equations are

$$\begin{aligned} \Lambda^0{}_0 &= \cosh\theta = \Lambda^1{}_1 && (11.37) \\ \Lambda^1{}_0 &= -\sinh\theta = \Lambda^0{}_1 && (11.38) \\ & && (11.39) \end{aligned}$$

$$\Lambda = \begin{pmatrix} \cosh\theta & -\sinh\theta & 0 & 0 \\ -\sinh\theta & \cosh\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

θ is the rapidity. Computation of θ: The origin moves with $\mathbf{v}$t ($\mathbf{x}' = 0$ corresponds to $\mathbf{x} = \mathbf{v}t$)

$$\begin{aligned} x' = 0 &= \Lambda^1{}_0 ct + \Lambda^1{}_1 vt && (11.40) \\ &\rightarrow \Lambda^1{}_0 = -\Lambda^1{}_1 \frac{v}{c} && (11.41) \\ &\rightarrow \sinh\theta = \frac{v}{c}\cosh\theta && (11.42) \\ &\rightarrow \tanh\theta = \frac{v}{c} && (11.43) \end{aligned}$$

$$\cosh\theta = \frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \gamma \quad (11.44)$$

$$\sinh\theta = \frac{v}{c}\frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \beta\gamma \quad (11.45)$$

$$\Lambda = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

11.2 Relativistic wave-equations

The derivative is a 4-vector

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right) \quad (11.46)$$

$$\partial^\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right) \quad (11.47)$$

A lorentz-invariant differential-operator could be a scalar product $\sum_\mu \partial^\mu \partial_\mu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta = \Box$. A possible relativistic wave-equation might be

$$\Box\phi = 0 \quad (11.48)$$

which is the **massless Klein-Gordan-equation**.

Definition 7. ***Eigentime*** *τ: The time in the rest-frame of a particle.*

$$ds^2 = c^2 d\tau^2 = c^2 dt^2 - d\mathbf{x}^2 = (c^2\mathbf{v}^2)dt^2 \quad (11.49)$$

$$d\tau = \sqrt{1-\left(\frac{v}{c}\right)^2}\gamma^{-1}dt \quad (11.50)$$

$$\tau = \int_{t_1}^{t_2} \gamma^{-1}dt \quad (11.51)$$

Definition 8. *The* ***4-momentum*** *is:*

$$p^\mu = m_0\frac{dx^\mu}{d\tau} = m_0\gamma\frac{x^\mu}{dt} = m_0\gamma(c, \boldsymbol{v}) \quad (11.52)$$

m_0 is the ***rest-mass***

For small v we get the well-known non-relativistiv relations:

$$\begin{aligned} m &= m_0\gamma & (11.53)\\ &\approx m_0 + \frac{1}{2}m_0\frac{v^2}{c^2} + ... & (11.54)\\ E = mc^2 &\approx m_0c^2 + \frac{1}{2}m_0\mathbf{v}^2 & (11.55)\end{aligned}$$

Finally we have the relativistic **Energy-momentum-relation**

$$\begin{aligned} E &= c\sqrt{m_0^2c^2 + \mathbf{p}^2} \\ &\approx \begin{cases} m_0c^2 + \frac{\mathbf{p}^2}{2m_0} + ... & |\mathbf{p}| << mc \\ c|\mathbf{p}| + ... & |\mathbf{p}| >> mc \end{cases}\end{aligned}$$

From this Energy-momentum-relation we can conclude a massive relativistic wave-equation.

$$\begin{aligned} \mathbf{p} &= \frac{\hbar}{i}\nabla & (11.56)\\ E &= i\hbar\frac{\partial}{\partial t} & (11.57)\end{aligned}$$

$$\begin{aligned} E^2 - c^2\mathbf{p}^2 &= -\hbar^2\frac{\partial^2}{\partial t^2} + \Delta = m_0^2c^4 & (11.58)\\ &\leftrightarrow \; c^2\hbar^2\left(-\frac{1}{c}\frac{\partial^2}{\partial t^2} + \Delta - \frac{m_0c^2}{\hbar^2}\right) = 0 & (11.59)\end{aligned}$$

And hence

$$\left(\Box + \left(\frac{m_oc}{\hbar}\right)^2\right)\phi = 0 \qquad (11.60)$$

the **massive Klein-Gordan-equation**.
These equations have certain problems since they are of second order in time. Therfore one must look for a relativistic wave-equation that is of first order in time. Two possibilities arise to do this

1. We could either take the squareroot

$$\sqrt{\Box + \left(\frac{m_oc}{\hbar}\right)^2} \qquad (11.61)$$

2. Or we could consider linear combinations

$$\sum_\mu \gamma^\mu\partial_\mu \qquad (11.62)$$

such that

$$\left(\sum_{\mu} \gamma^{\mu} \partial_{\mu}\right)^2 = \sum_{\mu} \partial^{\mu} \partial_{\mu} \tag{11.63}$$

the γ^{μ} are the so-called *Dirac-Matrices*.

11.3 Dirac equation

By: Andreas Bick

Das Ziel ist es eine Lorentz kovariante Schrödinger Gleichung zu finden. Der erste Kandidat dafür ist die Klein-Gordon Gleichung. Damit man ψ als Wellenfunktion interpretieren kann müsste die Klein-Gordon Gleichung eine Kontinuitätsgleichung erfüllen. Wir erinnern uns, dass im nichtrelativistischen Fall die Gleichung

$$\partial_t \rho + \vec{\nabla}\vec{j} = 0, \qquad \rho = \psi^*\psi \geq 0, \qquad \vec{j} = \frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)$$

sichert das

$$\partial_t \int \rho \mathrm{d}^3x = \partial_t \int |\psi(\vec{x},t)|^2 \, \mathrm{d}^3x = 0.$$

Dadurch haben wir eine sinnvolle Wahrscheinlichkeitsinterpretation. Nun versuchen wir für die KG Gleichung ein ρ und $\vec{j}$ zu finden. Dazu betrachten wir KG mit ψ^* multipliziert und die hermitisch konjugierte Gleichung.

$$\begin{aligned}
& \psi^*\left(\Box + \left(\frac{mc}{\hbar}\right)^2\right)\psi = 0, \qquad \psi\left(\Box + \left(\frac{mc}{\hbar}\right)^2\right)\psi^* = 0 \\
\Rightarrow \quad & \psi^*\Box\psi - \psi\Box\psi^* = 0 \\
\Leftrightarrow \quad & \frac{1}{c}\partial_t\left(\psi^*\partial_t\psi - \psi\partial_t\psi^*\right) - c\vec{\nabla}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)
\end{aligned}$$

Also können wir ρ und $\vec{j}$ wählen.

$$\rho = -\frac{\hbar}{2mic^2}\left(\psi^*\partial_t\psi - \psi\partial_t\psi^*\right), \qquad \vec{j} = \vec{j}_{\text{non rel.}}$$

Das Problem ist, dass ρ nun nicht mehr positiv definit ist und wir damit ψ nicht als Wellenfunktion interpretieren können.

Unser zweiter Versuch ist die Dirac Gleichung. Wir wählen den Ansatz:

$$i\hbar\partial_t\psi - H\psi = 0, \qquad H = -i\hbar c\vec{\alpha}\vec{\nabla} + \beta mc^2$$

mit $\vec{\alpha}, \beta$ konstant aber unbekannt. Wir fordern noch das ψ die Klein-Gordon Gleichung erfüllt. Der Sinn dieser Forderung wird klar wenn wir $E = i\hbar\partial_t$ und $\vec{p} = -i\hbar\vec{\nabla}$ in $E^2 - cp^2 - m^2c^4 = 0$ einsetzen, was uns genau die Klein Gordon Gleichung gibt. ψ erfüllt damit also die relativistische Energie-Impuls Beziehung.

Wir wenden nun $i\hbar\partial_t$ auf unseren Ansatz an.

$$(i\hbar)^2\partial_t^2\psi - HH\psi = 0 \propto \left(\Box + \left(\frac{mc}{\hbar}\right)^2\right)\psi = 0$$

Die Konstante wird so gewählt das der erste Term übereinstimmt.

$$\begin{aligned}(i\hbar)^2\partial_t^2 - HH &= (i\hbar)^2\partial_t^2 - (-i\hbar c\vec{\alpha}\vec{\nabla} + \beta mc^2)(-i\hbar c\vec{\alpha}\vec{\nabla} + \beta mc^2) \\ &= (i\hbar)^2\partial_t^2 - \big((i\hbar c)^2\alpha^i\alpha^j\partial_i\partial_j - i\hbar c\alpha^i\partial_i\beta mc^2 - i\hbar c\beta mc^2\alpha^j\partial_j + \beta^2(mc^2)^2\big) \\ &\overset{!}{=} -\hbar^2c^2\left(\frac{1}{c^2}\partial_t^2 - \partial^i\partial_i + \left(\frac{mc}{\hbar}\right)^2\right)\end{aligned}$$

Nun gehen wir Ordnung für Ordnung in den Ableitungen durch.

(1)

$$\begin{aligned}(\hbar c)^2\alpha^i\alpha^j\partial_i\partial_j &= \hbar^2c^2\partial^i\partial_i \\ \Leftrightarrow \frac{1}{2}(\alpha^i\alpha^j + \alpha^j\alpha^i)\partial_i\partial_j &= \delta^{ij}\partial_i\partial_j \\ \Rightarrow \frac{1}{2}(\alpha^i\alpha^j + \alpha^j\alpha^i) &= \delta^{ij}\mathbf{1}\end{aligned}$$

(2)

$$\begin{aligned}-i\hbar cmc^2\alpha^i\partial_i + \beta\alpha^i\partial_i &= 0 \\ \Rightarrow \alpha^i\beta + \beta\alpha^i &= 0\end{aligned}$$

(3)

$$\begin{aligned}\beta^2m^2c^4 &= \hbar^2c^2\frac{m^2c^2}{\hbar^2} \\ \Rightarrow \beta^2 &= \mathbf{1}\end{aligned}$$

Bei (1) wurden verwendet dass nur der symmetrische Teil der Summe beiträgt, da $\partial_i\partial_j$ symmetrisch ist. Aus (2) folgt sofort, dass α^i und β keine Zahlen sein können. Nun noch einige weitere Eigenschaften von α^i und β.

$$H = -i\hbar c\alpha^i\partial_i + \beta mc^2$$

$$\begin{aligned}&\text{(i)} \quad H^\dagger = H \qquad \Rightarrow \beta^\dagger = \beta, \left(\alpha^i\right)^\dagger = \alpha^i \\ &\text{(ii)} \quad \mathrm{Sp}(\alpha^i) = \mathrm{Sp}(\beta) = 0\end{aligned}$$

Beweis von (ii):

$$\mathrm{Sp}(\alpha^i) \overset{(3)}{=} \mathrm{Sp}(\beta^2\alpha^i) \overset{\text{zyklisch}}{=} \mathrm{Sp}(\beta\alpha^i\beta) \overset{(2)}{=} -\mathrm{Sp}(\beta^2\alpha^i) = \mathrm{Sp}(\alpha^i)$$
$$\mathrm{Sp}(\beta) = \mathrm{Sp}(\underbrace{(\alpha^i)^2}_{=\mathbf{1}}\beta) = \mathrm{Sp}(\alpha^i\beta\alpha^i) = -\mathrm{Sp}((\alpha^i)^2\beta) = -\mathrm{Sp}(\beta)$$

Die erste Idee wären sicher die Pauli Matrizen $\vec{\sigma}$ mit

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

und

$$\frac{1}{2}\left(\sigma^i\sigma^j + \sigma^j\sigma^i\right) = \delta^{ij}.$$

Die Anzahl der positiven und negativen Eigenwerte muss gleich sein damit die Spur null ist. Also ist n gerade. $n = 2$ genügt nicht, denn $(\mathbf{1}, \sigma^i)$ enthalten nur drei antikummutierende Matrizen. Die kleinstmögliche Dimension ist also $n = 4$ die uns auch eine Lösung mit

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & -\mathbf{1}_{2\times 2} \end{pmatrix}$$

gibt. Nun können wir die Beziehungen (1) bis (3) nachrechnen:

(1)

$$\begin{aligned} \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma^j \\ \sigma^j & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma^j \\ \sigma^j & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} &= \begin{pmatrix} \sigma^i\sigma^j + \sigma^j\sigma^i & 0 \\ 0 & \sigma^i\sigma^j + \sigma^j\sigma^i \end{pmatrix} \\ &= 2\delta^{ij}\begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & \mathbf{1}_{2\times 2} \end{pmatrix} \end{aligned}$$

(2)

$$\begin{aligned} &\begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}\begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & -\mathbf{1}_{2\times 2} \end{pmatrix} + \begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & -\mathbf{1}_{2\times 2} \end{pmatrix}\begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -\sigma^i \\ \sigma^i & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} = 0 \end{aligned}$$

(3)

$$\beta^2 = \mathbf{1}$$

Da wir jetzt die Form von α^i und β kennen wissen wir, dass ψ ein vierdimensionaler Vektor oder auch Viererspinor ist mit

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi_a &= \sum_b H_{ab}\psi_b \\ H_{ab} &= -i\hbar c\alpha^i_{ab}\partial_i + \beta_{ab}mc^2 \\ \left(\Box + \left(\frac{mc}{\hbar}\right)^2\right)\psi_a &= 0 \end{aligned}$$

Wir definieren noch den hermitisch adjugierten Spinor $\psi^\dagger$

$$\psi^\dagger \equiv (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*)$$

Um auf die Kontinuitätsgleichung zu kommen multiplizieren wir die Dirac Gleichung mit $\psi^\dagger$

$$i\hbar \sum_{a=1}^{4} \psi^\dagger a \partial_t \psi_a = \sum_{a,b=1}^{4} \psi_a^\dagger H_{ab} \psi_b = -i\hbar c \psi^\dagger \alpha^i \partial_i \psi + \psi^\dagger \beta mc^2 \psi$$

und betrachten die hermitisch Konjugierte Gleichung:

$$-i\hbar c \frac{\partial \psi^\dagger}{\partial t} \psi = i\hbar (\partial_i \psi^\dagger)(\alpha^i)^\dagger \psi + mc^2 \psi^\dagger \beta^\dagger \psi$$

Subtrahiert man diese Gleichungen voneinandern so erhält man einen Ausdruck der Form:

$$\partial_t \left(\psi^\dagger \psi\right) = c \partial_i \left(\psi^\dagger \alpha^i \psi\right)$$

Vergleicht man dieses nun mit der Kontinuitätsgleichung

$$\partial_t \rho + \vec{\nabla} \vec{j} = 0$$

so erfüllt die Gleichung dies genau für

$$\rho = \psi^\dagger \psi \qquad \text{und} \qquad \vec{j} = c \psi^\dagger \vec{\alpha} \psi$$

mit der gesuchten positiv definiten Wahrscheinlichkeitsdichte ρ.

11.4 Lösung der Dirac Gleichung

`By: Andreas Bick`

Im folgenden wollen wir die Lösungen der Dirac Gleichung suchen.

$$\left(-i\gamma^\mu \partial_\mu + \frac{mc}{\hbar}\mathbf{1}\right)\psi = 0$$

Zuerst betrachten wir ein Teilchen in Ruhe, also

$$\vec{p} = 0, \qquad \frac{\partial \psi}{\partial x^i} = 0.$$

Setzen wir dies ein so erhalten wir die einfach lösbare Gleichung

$$\left(-i\gamma^0 \partial_0 + \frac{mc}{\hbar}\mathbf{1}\right)\psi = 0.$$

Die Lösung können wir sofort hinschreiben mit

$$\psi = U \cdot e^{i\lambda \frac{mc}{\hbar} x_0}, \qquad U = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}, \qquad \partial_0 U = 0$$

$$\begin{aligned} \left(\gamma^0 \lambda \frac{mc}{\hbar} + \frac{mc}{\hbar}\mathbf{1}\right)\psi &= 0 \\ \left(\lambda\gamma^0 + \mathbf{1}\right)\psi &= 0 \end{aligned}$$

Da γ^0 im unteren rechten Block negativ ist kann man die Lösungen in der Form

$$\psi^+ = U_r e^{-i\frac{mc}{\hbar}x_0}, \qquad U_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad U_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\psi^- = V_r e^{i\frac{mc}{\hbar}x_0}, \qquad V_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad V_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Man kann die Viererspinoren auch durch zwei Bispinoren darstellen, zum Beispiel mit den bekannten Dirac Spinoren.

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\text{z.B.} \qquad U_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \chi_1 \\ 0 \\ 0 \end{pmatrix}$$

Vergleicht man dieses Ergebnis jetzt mit der nicht relativistischen Quantenmechanik stößt man auf das Problem das es Lösungen mit negativen Energien auftreten. Wir schreiben E und t um mit $ct = x_0$ und $E = mc^2$

$$\Psi(\vec{x}, t)_{\text{n rel}} = \psi(\vec{x}) e^{-i\frac{Et}{\hbar}} = \psi(\vec{x}) e^{-i\frac{mc}{\hbar}x^0}$$

Bei ψ^+ handelt es sich also um Lösungen positiver Energie, bei ψ^- um Lösungen negativer Energie.

Als zweites lösen wir die Dirac Gleichung für $\vec{p} \neq 0$ Dazu wählen wir den Ansatz

$$\psi^+ = U_r(k) e^{ik_\mu x^\mu} \qquad \text{und} \qquad \psi^- = V_r(k) e^{-ik_\mu x^\mu}$$

Wir werden werden jetzt prüfen ob der Ansatz die Klein Gordon Gleichung erfüllt. Für den Vierervektor k_μ gilt

$$k_\mu x^\mu = k_0 x^0 - \vec{k}\vec{x}, \qquad k_0(p) = \frac{E}{c\hbar} = \frac{\sqrt{c^2\vec{p}^2 + m^2c^4}}{c\hbar}$$

Setzen wir den Ansatz in die KG Gleichung ein:

$$\left(\Box + \left(\frac{mc}{\hbar}\right)^2\right)\psi^\pm = \left((\pm ik_\mu)(\pm ik^\mu) + \left(\frac{mc}{\hbar}\right)^2\right)\psi^\pm = \left(-k^\mu k_\mu + \left(\frac{mc}{\hbar}\right)^2\right)\psi^\pm$$

Für das Produkt der Viererwellenzahlvektoren gilt nun

$$k_\mu k^\mu = k_0 k^0 - \vec{k}\cdot\vec{k} = \frac{c^2\vec{p}^2 + m^2c^4}{c^2\hbar^2} - \frac{\vec{p}\cdot\vec{p}}{\hbar^2} = \left(\frac{mc}{\hbar}\right)^2$$

Der Term hebt sich also genau mit dem vorhandenen raus, damit ist die Klein Gorgon Gleichung erfüllt. Der Exponent ist gerade so gewählt das dies gilt.

Nun setzen wir den Ansatz in die Dirac Gleichung ein

$$\left(-i\gamma^\mu\partial_\mu - \frac{mc}{\hbar}\right)\psi^\pm = \left(-i\gamma^\mu\left(\pm ik_\mu\right) - \frac{mc}{\hbar}\right)\psi^\pm$$

Also erhalten wir einen Satz von algebraischen Gleichungen der Form

$$\begin{aligned} \left(\gamma^\mu k_\mu - \frac{mc}{\hbar}\right) U_r &= 0 \\ \left(\gamma^\mu k_\mu + \frac{mc}{\hbar}\right) V_r &= 0 \end{aligned}$$

Um die Gleichungen umzuschreiben betrachten wir

$$\begin{aligned}\left(\gamma^\mu k_\mu - \frac{mc}{\hbar}\right)\left(\gamma^\nu k_\nu + \frac{mc}{\hbar}\right) &= \gamma^\mu\gamma^\nu k_\mu k_\nu - \frac{mc}{\hbar}\gamma^\nu k_\nu + \gamma^\mu k_\mu \frac{mc}{\hbar} - \left(\frac{mc}{\hbar}\right)^2 \\ &= \frac{1}{2}\left(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu\right) k_\mu k_\nu - \left(\frac{mc}{\hbar}\right)^2 \\ &= \eta^{\mu\nu} k_\mu k_\nu - \left(\frac{mc}{\hbar}\right)^2 = k_\mu k^\mu - \left(\frac{mc}{\hbar}\right)^2 = 0\end{aligned}$$

Dadurch können wir die Lösungen jetzt bis auf eine Normalisierung N_I

$$U_r = N_U\left(\gamma^\mu k_\mu + \frac{mc}{\hbar}\right)\begin{pmatrix}\chi_r\\0\\0\end{pmatrix}, \qquad V_r = N_V\left(-\gamma^\mu k_\mu + \frac{mc}{\hbar}\right)\begin{pmatrix}0\\0\\\chi_r\end{pmatrix}$$

Nun können wir die Gleichungen wieder umschreiben mit

$$\gamma^\mu k_\mu = \gamma^0 k_0 - \gamma^i k_i = \begin{pmatrix}\mathbf{1}k_0 & 0\\ 0 & -\mathbf{1}k_0\end{pmatrix} - \begin{pmatrix}0 & \sigma^i k_i\\ -\sigma^i k_i & 0\end{pmatrix} = \begin{pmatrix}\mathbf{1}k_0 & -\sigma^i k_i\\ \sigma^i k_i & -\mathbf{1}k_0\end{pmatrix}.$$

Daher gilt weiterhin

$$\gamma^\mu k_\mu \begin{pmatrix}\chi_r\\0\end{pmatrix} = \begin{pmatrix}k_0\chi_r\\ \sigma^i k_i \chi_r\end{pmatrix}$$

Durch diese Umformungen können wir nun einen Ausdruck für U_r und V_r angeben, aus dem wir dann die Normierungsfaktoren bestimmen können. Wir erhalten

$$\begin{aligned} U_r &= N_U \begin{pmatrix}\left(k_0 + \frac{mc}{\hbar}\right)\chi_r\\ \vec{k}\cdot\vec{\sigma}\chi_r\end{pmatrix} \\ V_r &= N_V \begin{pmatrix}\vec{k}\cdot\vec{\sigma}\chi_r\\ \left(k_0 + \frac{mc}{\hbar}\right)\chi_r\end{pmatrix}\end{aligned}$$

Nun wollen wir den Normierungsfaktor, z.B. N_U berechnen. Für den adjungierten Spinor gilt

$$\overline{\psi} \equiv \psi^\dagger\gamma^0.$$

Also erhalten wir für unsere Lösungen

$$\overline{\psi^{(+)}} = \left(\psi^{(+)}\right)^\dagger \gamma^0 = U_r^\dagger e^{ik_\mu x^\mu}\gamma^0 = \overline{U_r} e^{ik_\mu x^\mu}$$

und analog dazu

$$\overline{\psi^{(-)}} = \overline{V_r} e^{-ik_\mu x^\mu}.$$

Betrachtet wir nun $\overline{U_r}$.

$$\overline{U_r} = U_r^\dagger \gamma^0 = N_U^\dagger (\chi_r, 0) \left(\overbrace{(\gamma^\mu)^\dagger}^{=\gamma^0\gamma^\mu\gamma^0} k_\mu + \frac{mc}{\hbar} \right) \gamma^0 = N_U^\dagger \overbrace{(\chi_r, 0)\,\gamma^0}^{=(\chi_r,0)} \left(\gamma^\mu k_\mu + \frac{mc}{\hbar} \right)$$

Um die Normierung zu berechnen betrachten wir

$$\begin{aligned} \overline{U_r} U_s &= |N_U|^2 (\chi_r, 0) \left(\gamma^\mu k_\mu + \frac{mc}{\hbar} \right) \left(\gamma^\mu k_\mu + \frac{mc}{\hbar} \right) \begin{pmatrix} \chi_s \\ 0 \end{pmatrix} \\ &= |N_U|^2 (\chi_r, 0) \frac{2mc}{\hbar} \left(\gamma^\mu k_\mu + \frac{mc}{\hbar} \right) \begin{pmatrix} \chi_s \\ 0 \end{pmatrix} \end{aligned}$$

Betrachten wir nun

$$(\chi_r, 0)\,\gamma^\mu \begin{pmatrix} \chi_s \\ 0 \end{pmatrix} = (\chi_r, 0)\,\gamma^0 \begin{pmatrix} \chi_s \\ 0 \end{pmatrix} = \chi_r \chi_s = \delta_{rs}$$

Von den γ^μ gibt nur γ^0 einen Beitrag, da alle γ^i offdiagonal sind. Also ergibt sich für die Normierung:

$$\begin{aligned} \overline{U_r} U_s &= \underbrace{2|N_U|^2 \frac{mc}{\hbar} \left(k_0 + \frac{mc}{\hbar} \right)}_{\stackrel{!}{=}1} \delta_{rs} \\ \Rightarrow N_U &= \frac{1}{\sqrt{2\frac{mc}{\hbar}\left(\frac{mc}{\hbar} + \frac{E}{c\hbar}\right)}} \end{aligned}$$

12 Coupling of the Dirac equation to the electromagnetic field

Starting from the free-particle Dirac equation

$$\left(-i\gamma^\mu p_\mu + \frac{mc}{\hbar}\right)\psi = 0 \Longleftrightarrow i\hbar\frac{\partial\psi}{\partial t} = \left(-ic\hbar\alpha^i p_i + \beta mc^2\right)\psi$$

with $p_i = -i\hbar\partial_i$, we couple the particle to the electromagnetic field by substituting for the momentum $\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}$, with the vector potential $\vec{A}$, and adding the term $e\phi\psi$ for the energy of the particle in the electric potential ϕ:

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= \left(c\alpha^i(p_i - \frac{e}{c}A_i) + \beta mc^2 + e\phi\right)\psi \\ &= \left(-i\hbar c\alpha^i(\partial_i - \frac{ie}{\hbar c}A_i) + \beta mc^2 + e\phi\right)\psi \end{aligned}$$

Writing this again in terms of γ-matrices with $\beta = \gamma^0$, $\alpha^i = \gamma^0\gamma^i$, we get by multiplying the equation with γ^0 and dividing by $\hbar c$,

$$\left(-i\gamma^0\partial_0 - i\gamma^i(\partial_i - \frac{ie}{\hbar c}A_i) + \gamma^0\frac{e}{\hbar c}\phi + \frac{mc}{\hbar}\right)\psi$$

$$\Longleftrightarrow \left(-i\gamma^\mu(\partial_\mu - \frac{ie}{\hbar c}A_\mu) + \frac{m}{\hbar c}\right)\psi = 0$$

where we introduced the four vector potential $A_\mu = (\phi, -\vec{A})$. This we could have got in the first place if we had replaced $\partial_\mu \to \partial_\mu - \frac{ie}{\hbar c}A_\mu$ in the covariant form of the Dirac equation.
In the following we now want to find the non-relativistic approximation of the Dirac equation coupled to the electromagnetic field.

$$i\hbar\frac{\partial\psi}{\partial t} = \left(c\alpha^i\pi_i + \beta mc^2 + e\phi\right)\psi, \qquad \pi_i = p_i - \frac{e}{c}A_i$$

Therefore we start with an ansatz for the solution of this equation,

$$\psi = e^{-\frac{imc^2}{\hbar}t}\begin{pmatrix}\varphi \\ \chi\end{pmatrix}$$

where φ and χ are supposed to be two-component spinors. Plugging this in and using the explicit form of the matrices $\beta = \begin{pmatrix}\mathbf{1} & 0 \\ 0 & -\mathbf{1}\end{pmatrix}$ and $\alpha^i =$

$\begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}$, we get

$$\begin{aligned} i\hbar\partial_t \begin{pmatrix} \varphi \\ \chi \end{pmatrix} &= i\hbar \left(-\frac{imc^2}{\hbar} e^{-\frac{imc^2}{\hbar}t} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} + e^{-\frac{imc^2}{\hbar}t} \begin{pmatrix} \partial_t\varphi \\ \partial_t\chi \end{pmatrix} \right) \\ &= \left(c \begin{pmatrix} \sigma^i\pi_i\chi \\ \sigma^i\pi_i\varphi \end{pmatrix} + e\phi \begin{pmatrix} \varphi \\ \chi \end{pmatrix} + mc^2 \begin{pmatrix} \varphi \\ -\chi \end{pmatrix} \right) e^{-\frac{imc^2}{\hbar}t} \end{aligned}$$

Bringing the first term in the upper line to the other side of the equation and cancelling the exponentials, we end up with (the two equations)

$$i\hbar \begin{pmatrix} \partial_t\varphi \\ \partial_t\chi \end{pmatrix} = c \begin{pmatrix} \sigma^i\pi_i\chi \\ \sigma^i\pi_i\varphi \end{pmatrix} + e\phi \begin{pmatrix} \varphi \\ \chi \end{pmatrix} + mc^2 \begin{pmatrix} 0 \\ -2\chi \end{pmatrix}$$

In the non-relativistic limit, $E \approx mc^2$, we neglect the terms

$$e\phi \ll mc^2, \qquad i\hbar\partial_t\chi \ll mc^2$$

>From the lower one of these equations we then simply get

$$0 = c\sigma^i\pi_i\varphi - 2mc^2\chi \Longrightarrow \chi = \frac{\sigma^i\pi_i}{2mc}\varphi,$$

which we can insert into the upper equation yielding

$$i\hbar\partial_t\varphi = c\sigma^i\pi_i\frac{\sigma^i\pi_i}{2mc}\varphi + e\phi\varphi$$

Recalling the algebra of the σ matrices, $\sigma^i\sigma^j = \delta^{ij} + i\epsilon^{ijk}\sigma^k$, this is

$$i\hbar\partial_t\varphi = \left(\frac{\pi^i\pi_i}{2m} + \frac{i}{2m}\epsilon^{ijk}\sigma_k\pi_i\pi_j + e\phi \right)\varphi$$

To evaluate the term $\epsilon^{ijk}\pi_i\pi_j$ we have to remind ourselves that in $\pi_i = p_i - \frac{e}{c}A_i$, $p_i = -i\hbar\partial_i$ is an operator, so

$$\begin{aligned} \epsilon^{ijk}\pi_i\pi_j &= \epsilon^{ijk}(-i\hbar\partial_i - \frac{e}{c}A_i)(-i\hbar\partial_j - \frac{e}{c}A_j) \\ &= \epsilon^{ijk}(-\hbar^2\partial_i\partial_j + \frac{i\hbar e}{c}(A_i\partial_j + (\partial_i A_j) + A_j\partial_i) + \frac{e^2}{c^2}A_iA_j) \end{aligned}$$

The first and the last term in this expression, and also, the first and the last term in the inner bracket vanish by virtue of the antisymmetry of ϵ^{ijk}. The remaining term, $\epsilon^{ijk}\partial_i A_j$, is the curl of the vector potential, which is, however, just the magnetic field B^k. What remains now is the the famous **Pauli equation**:

$$i\hbar\partial_t\varphi = \left(\frac{(p_i - \frac{e}{c}A_i)(p_i - \frac{e}{c}A_i)}{2m} - \frac{e\hbar}{2mc}\sigma^k B_k + e\phi\right)\varphi$$

If we now compare this to ordinary non-relativistic quantum mechanics of a particle in the electromagnetic field, where we have the Hamiltonian

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\phi = -\frac{\hbar^2}{2m}\Delta + \frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla} + \frac{e^2}{2mc^2}\vec{A}^2 + e\phi$$

in the Coulomb gauge $\vec{\nabla}\cdot\vec{A} = 0$, we get, for a constant magnetic field, for which the vector potential is given by $\vec{A} = \frac{1}{2}\vec{x}\times\vec{B}_0$,

$$H_0 = -\frac{\hbar^2}{2m}\Delta - \vec{\mu}\cdot\vec{B}_0 + \frac{e^2}{2mc^2}\vec{A}^2 + e\phi$$

since $(\vec{x}\times\vec{B})\cdot\vec{p} = -\vec{B}\cdot(\vec{x}\times\vec{p}) = -\vec{B}\cdot\vec{L}$, where $\vec{L} = \vec{x}\times\vec{p}$ is the orbital angular momentum operator and we have introduced the magnetic moment $\vec{\mu} = \frac{e}{2mc}\vec{L}$. To this we can add ad hoc a contribution to the magnetic moment coming from spin, $\vec{\mu}_{spin} = g\cdot\frac{e}{2mc}\vec{S}$, with the spin angular momentum operator $S = \frac{\hbar}{2}\vec{\sigma}$, in which we have to determine the numerical factor g (the so called Landé factor) from experiment (first conducted by Zeeman), which turns out to be approxiamtely $g \approx 2$. Our Hamiltonian becomes

$$H = H_0 - \vec{\mu}_{spin}\cdot\vec{B}_0 = H_0 - g\cdot\frac{e}{2mc}\frac{\hbar}{2}\vec{\sigma}\cdot\vec{B}$$

For this to match with the non-relativistic approximation of the Dirac equation, we must have $g = 2$, which seems to be good, but is not yet quite the right answer, which we will only get from quantum field theory.

13 Lösung der Dirac-Gleichung für das Coulomb-Potential $\Rightarrow$ relativistische Korrekturen des H-Atoms

In diesem Abschnitt wird die Dirac-Gleichung für ein Elektron im Coulomb-Potential <u>exakt</u> gelöst. Für die Energie werden wir zusätzlich zu dem Ausdruck $E \propto 1/n^2$, den wir bereits in der nichtrelativistischen Behandlung des Wasserstoffatoms (ohne Spin) exakt errechnen konnten, die Ruheenergie sowie die Feinstruktur-Korrekturen erhalten.
Der Dirac-Hamilton-Operator ergibt sich zu

$$H = c\vec{\alpha}\vec{\pi} + \beta mc^2 + e\,\Phi\mathbf{1} = \begin{pmatrix} mc^2 + e\,\Phi & c\vec{\sigma}\vec{\pi} \\ c\vec{\sigma}\vec{\pi} & -mc^2 + e\,\Phi \end{pmatrix} ,$$

wobei

$$\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A} \overset{\vec{A}=0}{=} \vec{p} \quad , \quad \Phi = -\frac{Ze}{r} .$$

Nach Separation der Zeitabhängigkeit der Lösung (Potential zeitunabhängig) $\Psi(\vec{x},t) = \mathrm{e}^{-\frac{iEt}{\hbar}}\psi(\vec{x})$ verbleibt

$$(H - E)\,\psi = 0 . \tag{13.1}$$

<u>Definition:</u> $\vec{J} := \vec{L}\cdot\mathbf{1} + \frac{\hbar}{2}\vec{\Sigma}$ Gesamtdrehimpuls , $\vec{\Sigma} := \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$

<u>Eigenschaft:</u> $[\vec{J}, H] = 0$

Beweis: Mit $[L_i, \phi] = [L_i, mc] = 0$ sowie $[\Sigma_i, \Phi] = 0$ verbleibt

$$[L_i, H] = c\alpha^j[L_i, p_j] = \mathrm{i}\,\hbar c\,\epsilon_{ijk}\alpha^j p^k = 0 \quad \text{sowie}$$

$$\frac{\hbar}{2}[\Sigma_i, H] = \frac{\hbar}{2}\big(c\underbrace{[\Sigma_i, \alpha_j]}_{=2\mathrm{i}\epsilon_{ijk}\alpha^k} p^j + mc^2\underbrace{[\Sigma_i, \gamma^0]}_{=0}\big) = \mathrm{i}\,\hbar c\,\epsilon_{ijk}\alpha^k p^j = 0$$

Wir können also gemeinsame Eigenzustände von H, $\vec{J}^2$ und J_z finden.
Die Eigenzustände von $\vec{J}^2$, J_z und $\vec{L}^2$ mit Gesamtdrehimpuls $j = l + 1/2$ und $j = l - 1/2$ sind Linearkombinationen der Produktzustände im 'Ketraum' bzw. in der Ortsdarstellung

$$|j = l + 1/2, m_j, l\rangle = a\,|l, m_l = m_j - 1/2\rangle\ |\uparrow\rangle + b\,|l, m_l = m_j + 1/2\rangle\ |\downarrow\rangle$$

$$\text{bzw.} \qquad \varphi^{(+)}_{j\,m_j} = a\,Y_{l,m_j-1/2}\begin{pmatrix}1\\0\end{pmatrix} + b\,Y_{l,m_j+1/2}\begin{pmatrix}0\\1\end{pmatrix}$$

und

$$|j = l - 1/2, m_j, l\rangle = b\,|l, m_l = m_j - 1/2\rangle\;|\!\uparrow\rangle - a\,|l, m_l = m_j + 1/2\rangle\;|\!\downarrow\rangle$$

$$\text{bzw.}\qquad \varphi^{(-)}_{j\,m_j} = b\,Y_{l,m_j-1/2}\begin{pmatrix}1\\0\end{pmatrix} - a\,Y_{l,m_j+1/2}\begin{pmatrix}0\\1\end{pmatrix}\;,$$

wobei $-j \leq m_j \leq j$ und mit den Clebsch-Gordan-Koeffizienten

$$a = \sqrt{\frac{l + m_j + 1/2}{2l+1}} \quad , \quad b = \sqrt{\frac{l - m_j + 1/2}{2l+1}}\;.$$

Zu jedem der Werte von j gibt es also zwei Pauli-Spinoren ($\varphi^{(+)}_{j\,m_j}$ und $\varphi^{(-)}_{j\,m_j}$), deren Bahndrehimpulse l sich gerade um 1 unterscheiden. Wir führen die Notation ein

$$\varphi^l_{j\,m_j} = \begin{cases}\varphi^{(+)}_{j\,m_j} & \text{für } l = j - \frac{1}{2}\\ \varphi^{(-)}_{j\,m_j} & \text{für } l = j + \frac{1}{2}\end{cases}$$

und machen den Ansatz für die (viererspinorwertige) Lösung der Dirac-Gleichung

$$\psi^l_{j\,m_j} = \begin{pmatrix}\frac{\mathrm{i}\,G_{lj}(r)}{r}\;\varphi^l_{j\,m_j}(\theta,\phi)\\ \frac{F_{lj}(r)}{r}\;(\vec{\sigma}\cdot\hat{x})\;\varphi^l_{j\,m_j}(\theta,\phi)\end{pmatrix} \qquad , \quad \hat{x} = \frac{\vec{x}}{|\vec{x}|} = \frac{\vec{x}}{r}\;. \tag{13.2}$$

$(\vec{\sigma}\cdot\hat{x})\;\varphi^l_{j\,m_j}$ ist auch Eigenfunktion zu $\vec{J}^2$ und J_z, da

$$[J_i, \vec{\sigma}\cdot\vec{x}] = \sigma_k[L_i, x^k] + \frac{\hbar}{2}[\sigma_i,\sigma_k]x^k = \mathrm{i}\hbar\,\epsilon_{ijk}\sigma^j x^k + 2\,\mathrm{i}\frac{\hbar}{2}\,\epsilon_{ikj}\sigma^j x^k = 0\;.$$

Im folgenden erweisen sich folgende Eigenschaften als nützlich:

$$\vec{J}^2 = \vec{L}^2 + \frac{\hbar^2}{4}\vec{\sigma}^2 + \hbar\,\vec{L}\cdot\vec{\sigma} \quad \Rightarrow \quad \hbar\,\vec{L}\cdot\vec{\sigma} = \vec{J}^2 - \vec{L}^2 - \frac{\hbar^2}{4}\vec{\sigma}^2$$

$$\begin{aligned}
\Rightarrow \quad \hbar\,\vec{L}\cdot\vec{\sigma}\varphi^l_{j\,m_j} &= \frac{\hbar^2}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)\varphi^l_{j\,m_j} \\
&= \frac{\hbar^2}{2}\begin{Bmatrix} l \\ -l-1 \end{Bmatrix}\varphi^l_{j\,m_j} \\
&= \frac{\hbar^2}{2}\begin{Bmatrix} -1 + (j+\frac{1}{2}) \\ -1 - (j+\frac{1}{2}) \end{Bmatrix}\varphi^l_{j\,m_j} \qquad \begin{cases} \text{für } j = l + \frac{1}{2} \\ \text{für } j = l - \frac{1}{2} \end{cases} \qquad \text{(i)}
\end{aligned}$$

$$(\vec{\sigma}\cdot\hat{x})(\vec{\sigma}\cdot\hat{x}) \overset{\sigma_i\sigma_j = \delta_{ij}\mathbf{1} + \mathrm{i}\,\epsilon_{ijk}\sigma^k}{=} \sigma_i\hat{x}^i\sigma_j\hat{x}^j = \mathbf{1}\,\delta_{ij}\hat{x}^i\hat{x}^j = \mathbf{1} \qquad \text{(ii)}$$

$$(\vec{\sigma}\cdot\hat{x})(\vec{\sigma}\cdot\vec{p}) = \sigma_i\hat{x}^i\sigma_j p^j \overset{\sigma_i\sigma_j = \delta_{ij}\mathbf{1} + \mathrm{i}\,\epsilon_{ijk}\sigma^k}{=} \hat{x}\cdot\vec{p} + \frac{\mathrm{i}}{r}\,\vec{L}\cdot\vec{\sigma} \qquad \text{(iii)}$$

$$\vec{x}\cdot\vec{p} = \frac{\hbar}{\mathrm{i}} r\frac{\partial}{\partial r} \qquad \text{(iv)}$$

$$\vec{p}\cdot\frac{\vec{x}}{r} = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x^i}\left(\frac{x^i}{r}\right) = \frac{\hbar}{\mathrm{i}}\left(\frac{2}{r} + \hat{x}^i\frac{\partial}{\partial x^i}\right) \qquad \text{(v)}$$

Hiermit berechnen wir

$$\begin{aligned}
&(\vec{\sigma}\cdot\vec{p})\,f(r)\,\varphi^l_{j\,m_j} \\
&\overset{\text{(ii)}}{=} (\vec{\sigma}\cdot\hat{x})(\vec{\sigma}\cdot\hat{x})(\vec{\sigma}\cdot\vec{p})\,f(r)\,\varphi^l_{j\,m_j} \\
&\overset{\text{(iii)}}{=} \frac{\vec{\sigma}\cdot\hat{x}}{r}\,(\vec{x}\cdot\vec{p} + \mathrm{i}\,\vec{L}\cdot\vec{\sigma})\,f(r)\,\varphi^l_{j\,m_j} \\
&\overset{\text{(i \& iv)}}{=} -\mathrm{i}\hbar\frac{\vec{\sigma}\cdot\hat{x}}{r}\left[r\frac{\partial}{\partial r} + 1 \mp \left(j + \frac{1}{2}\right)\right] f(r)\,\varphi^l_{j\,m_j} \quad \text{für } j = l \pm \frac{1}{2} \qquad \text{(a)}
\end{aligned}$$

und

$$\begin{aligned}
&(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\hat{x})\,f(r)\,\varphi^l_{j\,m_j} \\
&\overset{\text{(iii inv.)}}{=} \left(\vec{p}\cdot\hat{x} - \frac{\mathrm{i}}{r}\,\vec{L}\cdot\vec{\sigma}\right) f(r)\,\varphi^l_{j\,m_j} \\
&\overset{\text{(i \& iv)}}{=} -\frac{\mathrm{i}\hbar}{r}\left[r\frac{\partial}{\partial r} + 1 \pm \left(j + \frac{1}{2}\right)\right] f(r)\,\varphi^l_{j\,m_j} \quad \text{für } j = l \pm \frac{1}{2}\,. \qquad \text{(b)}
\end{aligned}$$

Einsetzen von (13.2) in die Dirac-Gleichung (13.1) führt hiermit auf das gekoppelte Paar (paulispinorwertiger) Differentialgleichungen

$$\left\{\begin{array}{l}\left(mc^2-\frac{Ze^2}{r}-E\right)\frac{\mathrm{i}G}{r}\,\varphi^l_{j\,m_j}+c(\vec\sigma\cdot\vec p)(\vec\sigma\cdot\hat x)\frac{F}{r}\,\varphi^l_{j\,m_j}=0\\ c(\vec\sigma\cdot\vec p)\frac{\mathrm{i}G}{r}\,\varphi^l_{j\,m_j}-\left(mc^2-\frac{Ze^2}{r}-E\right)\frac{F}{r}(\vec\sigma\cdot\hat x)\,\varphi^l_{j\,m_j}=0\end{array}\right.$$

$$\overset{(\mathrm{b}\,\&\,\mathrm{a})}{\Rightarrow}\left\{\begin{array}{l}\left(mc^2-\frac{Ze^2}{r}-E\right)\frac{\mathrm{i}G}{r}\,\varphi^l_{j\,m_j}-\frac{\mathrm{i}\hbar c}{r}\left[r\frac{\partial}{\partial r}+1\pm\left(j+\frac{1}{2}\right)\right]\frac{F}{r}\,\varphi^l_{j\,m_j}=0\\ -\frac{\mathrm{i}\hbar c}{r}\,(\vec\sigma\cdot\hat x)\,\varphi^l_{j\,m_j}\left[r\frac{\partial}{\partial r}+1\mp\left(j+\frac{1}{2}\right)\right]\frac{\mathrm{i}G}{r}-\left(mc^2-\frac{Ze^2}{r}-E\right)\frac{F}{r}(\vec\sigma\cdot\hat x)\,\varphi^l_{j\,m_j}=0\end{array}\right. ,$$

dessen winkelabhängiger Teil $\varphi^l_{j\,m_j}$ bzw. $(\vec\sigma\cdot\hat x)\,\varphi^l_{j\,m_j}$ sich nun eliminieren lässt:

$$\left\{\begin{array}{l}\left(mc^2-\frac{Ze^2}{r}-E\right)G(r)-\hbar c\left(\frac{\mathrm{d}F(r)}{\mathrm{d}r}\pm\left(j+\frac{1}{2}\right)\frac{F(r)}{r}\right)=0\\ \left(mc^2+\frac{Ze^2}{r}+E\right)F(r)-\hbar c\left(\frac{\mathrm{d}G(r)}{\mathrm{d}r}\mp\left(j+\frac{1}{2}\right)\frac{G(r)}{r}\right)=0\end{array}\right. \qquad (13.1')$$

Mit den Substitutionen

$$\alpha_1=mc^2+E\,,\quad \alpha_2=mc^2-E\,,\quad \sigma=\sqrt{\alpha_1\alpha_2}=\sqrt{m^2c^4-E^2}$$
$$\rho=r\frac{\sigma}{\hbar c}\,,\qquad k=\pm(j+\frac{1}{2})\,,\quad \gamma=\frac{Ze^2}{\hbar c}=Z\alpha\ \ (\alpha:\text{Feinstrukturkonst.})$$

schreibt sich (13.1′) als

$$\left\{\begin{array}{l}\left(\frac{\mathrm{d}}{\mathrm{d}\rho}+\frac{k}{\rho}\right)F-\left(\frac{\alpha_2}{\sigma}-\frac{\gamma}{\rho}\right)G=0\\ \left(\frac{\mathrm{d}}{\mathrm{d}\rho}-\frac{k}{\rho}\right)G-\left(\frac{\alpha_1}{\sigma}+\frac{\gamma}{\rho}\right)F=0\end{array}\right. .$$

Aus der Normierungsbedingung folgt, dass F und G sich für große ρ wie $\mathrm{e}^{-\rho}$ verhalten muss. Wir wählen daher

$$\begin{array}{lll}F(\rho)=f(\rho)\,\mathrm{e}^{-\rho} & \Rightarrow & F'(\rho)=(f'(\rho)-f(\rho))\,\mathrm{e}^{-\rho}\\ G(\rho)=g(\rho)\,\mathrm{e}^{-\rho} & \Rightarrow & G'(\rho)=(g'(\rho)-g(\rho))\,\mathrm{e}^{-\rho}\end{array}$$

und erhalten

$$\left\{\begin{array}{l}f'-f+\frac{kf}{\rho}-\left(\frac{\alpha_2}{\sigma}-\frac{\gamma}{\rho}\right)g=0\\ g'-g-\frac{kg}{\rho}-\left(\frac{\alpha_1}{\sigma}+\frac{\gamma}{\rho}\right)f=0\end{array}\right. .$$

Ansatz:

$$f(\rho)=\rho^s\sum_{\nu=0}^{\infty}a_\nu\rho^\nu\quad\Rightarrow\quad f'(\rho)=s\,\rho^{s-1}\sum_{\nu=0}^{\infty}a_\nu\rho^\nu+\rho^s\sum_{\nu=0}^{\infty}\nu\,a_\nu\rho^{\nu-1}$$
$$g(\rho)=\rho^s\sum_{\nu=0}^{\infty}b_\nu\rho^\nu\quad\Rightarrow\quad g'(\rho)=s\,\rho^{s-1}\sum_{\nu=0}^{\infty}b_\nu\rho^\nu+\rho^s\sum_{\nu=0}^{\infty}\nu\,b_\nu\rho^{\nu-1}$$

Wir suchen eine Rekursionsformel für a_ν und b_ν und betrachten dazu zunächst den Koefizienten von $\rho^{s+\nu-1}$:

$$\begin{cases} (s+\nu)a_\nu - a_{\nu-1} + ka_\nu - \frac{\alpha_2}{\sigma}b_{\nu-1} + \gamma b_\nu = 0 & (\star) \\ (s+\nu)b_\nu - b_{\nu-1} - kb_\nu - \frac{\alpha_1}{\sigma}a_{\nu-1} - \gamma a_\nu = 0 & (\star\star) \end{cases}$$

Für $\nu = 0$ erhalten wir

$$\begin{cases} (s+k)a_0 + \gamma b_0 = 0 \\ (s-k)b_0 - \gamma a_0 = 0 \end{cases} .$$

Dies sind zwei Gleichungen für zwei Unbekannte. Nichttriviale Lösungen $(a_0, b_0 \neq 0)$ existieren bei verschwindendem charakteristischen Polynom:

$$(s+k)(s-k) + \gamma^2 = 0 \quad \Rightarrow \quad s = \pm\sqrt{k^2 - \gamma^2}$$

Da die Lösung bei $\rho = 0$ regulär bleiben muss, wählen wir die positive Wurzel für s.
Nun betrachten wir die Linearkombination $\sigma \cdot (\star) \; - \; \alpha_2 \cdot (\star\star)$ und erhalten:

$$\left(\sigma(s+\nu+k) + \alpha_2\gamma\right) a_\nu - \left(\alpha_2(s+\nu-k) - \sigma\gamma\right) b_\nu = 0 \tag{13.3}$$

Für große ν reduziert sich diese Gleichung auf

$$\sigma\nu a_\nu - \alpha_2\nu b_\nu = 0 \quad \Rightarrow \quad a_\nu = \frac{\alpha_2}{\sigma} b_\nu$$

Hiermit kann in $(\star\star)$ bzw. $(\star)$ das b_ν bzw. a_ν eliminiert werden und wir erhalten im Limes $\nu \to \infty$ die Rekursionsformeln

$$a_\nu = \frac{2}{\nu}\, a_{\nu-1}$$

$$b_\nu = \frac{2}{\nu}\, b_{\nu-1}$$

Damit folgt

$$\sum_{\nu=0}^{\infty} a_\nu \rho^\nu \propto \sum_{\nu=0}^{\infty} b_\nu \rho^\nu \propto \sum_{\nu=0}^{\infty} \frac{(2\rho)^2}{\nu\,!} = \mathrm{e}^{2\rho} \overset{\rho\to\infty}{\longrightarrow} \infty ,$$

d.h. die Reihe verhält sich asymtotisch wie $\mathrm{e}^{2\rho}$ und somit $F(\rho)$ und $G(\rho)$ wie e^{ρ}.
Damit die Lösungen für große ρ beschränkt bleiben, müssen die Reihen bei

einer Zahl $\nu = N$ abbrechen und wir erhalten Polynome[1] vom Grad N. Es sei also

$$a_{N+1} = b_{N+1} = 0 \ .$$

Für $\nu = N+1$ erhalten wir damit aus $(\star)$[2] die Abbruchbedingung:

$$-a_N - \frac{\alpha_2}{\sigma} b_N = 0$$

Dies setzen wir mit $\nu = N$ in (13.3) ein und erhalten:

$$\begin{aligned} & a_N[\sigma(s+N+k) + \alpha_2\gamma) + \frac{\sigma}{\alpha_2}(\alpha_2(s+N-k) - \sigma\gamma)] = 0 \\ \Rightarrow \quad & 2\sigma(s+N) + \gamma(\underbrace{\alpha_2 - \alpha_1}_{=-2E}) = 0 \quad \Rightarrow \quad 2\sqrt{m^2c^4 - E^2}\,(s+N) = 2\gamma E \end{aligned}$$

$$\Longrightarrow \quad E = mc^2 \left(1 + \frac{\gamma^2}{(s+N)^2}\right)^{-\frac{1}{2}}$$

Man nennt $N = 0, 1, 2, ...$ die radiale Quantenzahl.
Führen wir die Hauptquantenzahl $n = N + |k|\,,\ |k| = j + 1/2$ ein, so erhalten wir als exaktes Ergebnis für die Energien des H-Atoms aus der Dirac-Gleichung schließlich

$$E = mc^2 \left[1 + \left(\frac{Z\alpha}{n - \left(j+\frac{1}{2}\right) + \sqrt{\left(j+\frac{1}{2}\right)^2 - (Z\alpha)^2}}\right)^2\right]^{-\frac{1}{2}} . \qquad (13.4)$$

Entwicklung von E aus (13.4) für $(Z\alpha) \ll 1$:

$$E = mc^2 \left[\underbrace{1}_{\text{Ruheenergie}} - \underbrace{\frac{(Z\alpha)^2}{2n^2}}_{\text{nichtrel. H-Atom}} - \underbrace{\frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right)}_{\text{Feinstrukturaufspaltung}} + \mathcal{O}[(Z\alpha)^6] \right]$$

[1]Bei der Lösung der Radialgleichung im nichtrelativistischen Fall (aus der Schrödingergleichung) befanden wir uns in einer ähnlichen Situation. Dies führte dort zu den Laguerre-Polynomen.

[2]$(\star\star)$ ergibt dieselbe Gleichung.

Der zweite Term in dieser Entwicklung unseres Ergebnisses in $(Z\alpha)$ ist der Ausdruck, den wir bereits in der nichtrelativistischen Behandlung des Wasserstoffatoms (ohne Spin) errechnet haben.
Der dritte Term entspricht genau den Korrekturen der Feinstruktur, die sich in der schrödigerschen Quantemechanik durch störungstheoretische Berechnungen ergeben und sowohl die relativistischen kinetischen Korrekturen als auch die Spin-Bahn-Kopplung (bzw. den Darwin-Term für $l = 0$) umfassen.

14 Introduction to Quantum Field Theory

14.1 Classical Field Theory

In this chapter we will introduce some ideas of the quantum theory of fields which will be developed and discussed more fully in next term's course on quantum field theory.

To start with we will discuss classical field theory and particularly the action principle or Hamiltonian principle which leads to the Euler-Lagrange equations for fields.
Let $\phi_r(x)$, $r = 1, \dots, N$, be a collection of N fields depending on space and time. (From now on we use a notation in which x stands for $x = (x^\mu) = (t, \vec{x})$.) Examples would be a single scalar field $\phi(x)$, a Dirac 4-spinor $\psi_a(x)$ with $a = 1, \dots, 4$ or a gauge field $A_\mu(x)$ with $\mu = 0, \dots, 3$. Also let $\mathcal{L} = \mathcal{L}(\phi_r, \partial_\mu \phi_r)$ be a *Lagrangian desity* which depends on the fields and their first derivatives, such that the action S is given by

$$S = \int_V d^4x \, \mathcal{L}(\phi_r, \partial_\mu \phi_r) \tag{14.1}$$

where again we have put the system in a box of a finite spacetime volume V. (This constraint will be relaxed next term where we will consider action intergrals over all spacetime). Sometimes it is useful to talk about the Lagrangian L and not its density. They are related by $L = \int d^3x \, \mathcal{L}$ such that the action becomes

$$S = \int dt \, L \tag{14.2}$$

which is the familiar form we know from classical mechanics.

As one does in mechanics we now postulate that S has stationary points where the variation of S vanishes:

$$\delta S = 0 \quad \text{for} \quad \phi_r \longrightarrow \phi_r + \delta\phi_r \, . \tag{14.3}$$

The variation is set to zero on the boundary of the volume V, $\delta\phi_r|_{\partial V} = 0$, where ∂V denotes the boundary of V. We get

$$0 = \delta S = \int_V d^4x \sum_{r=1}^{N} \left(\frac{\partial \mathcal{L}}{\partial \phi_r} \, \delta\phi_r + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} \, \delta(\partial_\mu \phi_r) \right) \tag{14.4}$$

where (in complete analogy to classical mechanics) we treated the fields ϕ_r and their derivatives $\partial_\mu \phi_r$ as independent variables. We also demand

$$\delta(\partial_\mu \phi_r) = \partial_\mu (\delta\phi_r) \tag{14.5}$$

and thus rewrite (14.4) using the Leibnitz rule on the second term in the integral. We get

$$0 = \int_V d^4x \sum_{r=1}^{N} \left[\frac{\partial \mathcal{L}}{\partial \phi_r} \delta\phi_r + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} \delta\phi_r \right) - \left(\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} \right) \delta\phi_r \right] . \tag{14.6}$$

The integral of the middle term vanishes by virtue of Stoke's theorem and the constraint that $\delta\phi_r$ be zero at the boundary:

$$\int_V d^4x \, \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} \delta\phi_r \right) = \int_{\partial V} dS_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} \delta\phi_r = 0 \tag{14.7}$$

where dS_μ is the 3-dimensional normal surface element on ∂V. So from (14.6) we are left with

$$0 = \int_V d^4x \sum_{r=1}^{N} \left[\frac{\partial \mathcal{L}}{\partial \phi_r} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} \right] \delta\phi_r \tag{14.8}$$

for arbitrary and independent $\delta\phi_r$ for $r = 1, \ldots, N$. This is fullfilled if and only the bracket itself is already zero:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \phi_r} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_r)} = 0 \quad \text{for all } r = 1, \ldots, N \, .} \tag{14.9}$$

This set of N equations is known as the *Euler-Lagrange equations* for fields.

Again similar to classical mechanics we define the conjugate momentum to ϕ_r (strictly speaking it is a momentum *density*) to be

$$\pi_r := \frac{\partial \mathcal{L}}{\partial \dot{\phi}_r} \tag{14.10}$$

where we have written $\dot{\phi}_r$ to denote the field's time derivative $\partial_0 \phi_r$. The Hamiltonian of a classical field is then given by

$$H(\phi_r, \pi_r) \equiv \int d^3x \, \mathcal{H}(\phi_r, \pi_r) := \int d^3x \sum_{i=1}^{N} \left(\pi_r \dot{\phi}_r - \mathcal{L} \right) . \tag{14.11}$$

$\mathcal{H}$ is called the Hamiltonian density.

Example 1: Single Real Scalar Field

We take the Lagrangian density of a real scalar field ϕ to be

$$\mathcal{L}(\phi, \partial_\mu \phi) = \frac{1}{2}\left(\partial_\nu \phi \partial^\nu \phi - m^2\phi^2\right) . \tag{14.12}$$

In this formula we have chosen units in which

$$\boxed{\hbar = c = 1} \tag{14.13}$$

and for the rest of the course we will stick to this convenient convention. From the Lagrangian (14.12) we can compute

$$\frac{\partial \mathcal{L}}{\partial \phi} = -m^2\phi \tag{14.14}$$

and

$$\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} = \frac{1}{2}(\partial^\mu \phi + \partial^\mu \phi) = \partial^\mu \phi\,. \tag{14.15}$$

Puuting it all together the Euler-Lagrange equation for ϕ yields

$$-m^2\phi - \partial_\mu \partial^\mu \phi = 0 \quad \Longleftrightarrow \quad (\Box + m^2)\phi = 0 \tag{14.16}$$

which we immediately recognise as the Klein-Gordon equation. Therefore, (14.12) is sometimes also called the Klein-Gordon Langrangian. The conjugate momentum is

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi} \tag{14.17}$$

and hence the Hamiltonian density can be written as

$$\begin{aligned} \mathcal{H} = \pi\dot{\phi} - \mathcal{L} &= \dot{\phi}^2 - \frac{1}{2}\left(\dot{\phi}^2 - \vec{\nabla}\phi \cdot \vec{\nabla}\phi - m^2\phi^2\right) \\ &= \frac{1}{2}\left(\dot{\phi}^2 + \vec{\nabla}\phi \cdot \vec{\nabla}\phi + m^2\phi^2\right) . \end{aligned}$$

Example 2: Spinor Field

We now conduct the same steps with the so called Dirac Lagrangian whose Euler-Lagrange equations are the Dirac equations for the spinor field ψ and its conjugate $\bar{\psi} = \psi^\dagger \gamma^0$. The Langrangian (which we pull out of a hat) is given by

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi \tag{14.18}$$

and we compute

$$\frac{\partial \mathcal{L}}{\partial \psi} = -m\bar{\psi} \tag{14.19}$$

$$\frac{\partial \mathcal{L}}{\partial \bar{\psi}} = (i\gamma^\mu \partial_\mu - m)\psi \tag{14.20}$$

$$\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} = i\bar{\psi}\gamma^\mu \tag{14.21}$$

$$\frac{\partial \mathcal{L}}{\partial(\partial_\mu \bar{\psi})} = 0\,. \tag{14.22}$$

The Euler-Lagrange equation for $\bar{\psi}$ is just the Dirac equation

$$(i\gamma^\mu \partial_\mu - m)\,\psi = 0 \tag{14.23}$$

and the equation for ψ turns out to be

$$-m\bar{\psi} - \partial_\mu i\bar{\psi}\gamma^\mu = 0 \quad \Longleftrightarrow \quad i(\partial_\mu \bar{\psi})\gamma^\mu + m\bar{\psi} = 0 \tag{14.24}$$

which is the conjugate of (14.23). For the conjugate momenta we get

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\bar{\psi}\gamma^0 = i\psi^\dagger \tag{14.25}$$

and

$$\bar{\pi} = \frac{\partial \mathcal{L}}{\partial \dot{\bar{\psi}}} = 0\,. \tag{14.26}$$

The fact that $\bar{\pi}$ vanishes will be a problem that has to be taken care of when we come to quantising the theory next term. But for now we limit ourselves to classical field theory and to finish this section we write down what the Hamiltonian for the Dirac field is

$$\begin{aligned}
\mathcal{H} &= \pi\dot{\psi} + \bar{\pi}\dot{\bar{\psi}} - \mathcal{L} \\
&= i\psi^\dagger\dot{\psi} - \bar{\psi}(i\gamma^0\partial_0 + i\gamma^i\partial_i - m)\psi \\
&= -i\bar{\psi}\gamma^i\partial_i\psi + m\bar{\psi}\psi\,.
\end{aligned}$$