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e^+e^- Scattering to Hadrons Notes

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The τ-lepton is the only lepton heavy enough to decay into hadrons. It is an ideal candidate to perform a QCD analysis at low to intermediate energies[1], extracting and probing Standard model parameters like the strong coupling α_s. Due to it's W-Boson mediator it allows a study of the $q\bar{q}$ vector and axial vector current, whereas $e^+e^- \to \gamma^* \to (hadrons)$ scattering only covers the vector ones. For the tree level of the SM the tau decays into a ν_τ neutrino and a W-Boson, which then decays into either (ν_μ, μ) and (ν_e, e) lepton pairs or $(\bar{u}, d)$, and $(\bar{u}, s)$ quark pairs, as illustrated in Figure 1. Other quark pair generation is forbidden either due to the τ-mass of 1776.86 MeV [4] or the confinement of weak isospin (T_3)[2] Due to color confinement[3] the detected quark pairs are hadrons (pions, ρ mesons, kaons and others).

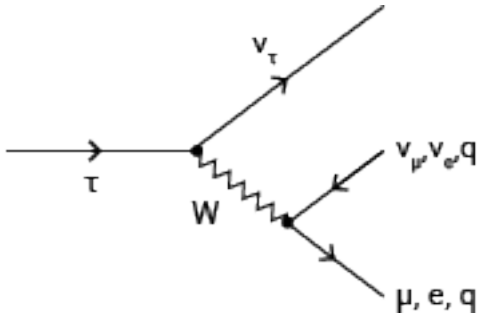

Figure 1. Standard Model τ decays.

The data is gathered via the ALEPH experiment in CERN and expressed through the ratio

$$R_\tau = \frac{\mathcal{B}_\tau}{\mathcal{B}_{e^-}} = \frac{\Gamma(\tau^- \to \text{hadrons}^- \nu_\tau)}{\Gamma(\tau^- \to e^- \bar{\nu}_e \nu_\tau)}, \tag{2.1}$$

which can be connected to the vacuum polarization $\Pi(s)$ of the W-Boson[4]. $\mathcal{B}_\tau$ and $\mathcal{B}_{e^-}$ are the branching fractions of the non strange hadronic and electronic decays and the Γs the respective decay rates.

Our aim is to match the experimental data with a theory model in a computer program to analyse and extract parameters of the SM. Therefore we will start connecting the experimental data with quantum field theory. Then describe the needed theory and experimental sides in detail. And lastly discuss the results.

[1] At high energies we have no valid theory because $\alpha_s >> 1$ for high-energies.

[2] E.g. the $(\bar{d}, u)$ pair would lead to $(\tau \to \nu_\tau + \bar{d} + u)$, which represents an inequality in terms of weak isopsin conservation $(-1/2 \neq +1/2 + 1/2 - 1/2)$.

[3] Quarks have never been seen as single particle, but only in compounds as mesons or baryons.

[4] Also refered to as the weak current two-point correlation function.

3 Theory

Starting point of our analysis will be the definition of the vector and axial vector QCD correlator

$$\Pi^{V/A}_{\mu\nu,ij}(p) \equiv i \int \mathrm{d}x e^{ipx} \langle \Omega | T\{ J^{V/A}_{\mu,ij}(x) J^{V/A}_{\nu,ij}(0)^\dagger \} | \Omega \rangle, \tag{3.1}$$

with $|\Omega\rangle$ being the physical vacuum and i, j representing the light quark flavours: up, down and strange[5]. The V and A currents are given by

$$J^{V/A}_{\mu,ij}(x) = [\bar{q}_j \gamma_\mu (\gamma_5) q_i](x). \tag{3.2}$$

The before introduced correlator can be decomposed in several ways starting by the standard longitudinal and transversal decomposition (omitting the flavour indices i, j from now on, if not necassary):

$$\begin{aligned} \Pi_{\mu\nu}(p)^{V/A} &= (p_\mu p_\nu - g_{\mu\nu} p^2) \Pi^{V/A,(1)}(p^2) + p_\mu p_\nu \Pi^{V/A,(0)}(p^2) \\ &= (p_\mu p_\nu - g_{\mu\nu} p^2) \Pi^{V/A,(1+0)}(p^2) + g_{\mu\nu} p^2 \Pi^{V/A,(0)}(p^2) \end{aligned} \tag{3.3}$$

, where the upper indice (1) denotes the transversal contribution and (0) the longitudinal one. Besides the Lorentz decomposition, the currents contributin to hadronic τ decays can also be decomposed according to their light quark flavour content:

$$\Pi^{(J)}_{V/A}(s) = |V_{ud}"^2 \left[\Pi^{V,(J)}_{ud}(s) + \Pi^{A,(J)}_{ud}(s) \right] + |V_{us}|^2 \left[\Pi^{V,(J)}_{us}(s) + \Pi^{A,(J)}_{us}(s) \right], \tag{3.4}$$

with V_{ij} being the corresponding elemtns of the Cabibbo-Kobayashi-Maskawas (CKM) quark-mixing matrix. Another useful decomposition of the V (A) correlator is the separation of vector (axial vector) and scalar (pseudoscalar) components

$$\begin{aligned} \Pi^{V/A}_{\mu\nu}(p) &= (p_\mu p_\nu - g_{\mu\nu} p^2) \Pi^{V/A}(p^2) \\ &\quad + \frac{g_{\mu\nu}}{p^2} (m_i \mp m_j)^2 \Pi^{S,P)}(p^2) + g_{\mu\nu} \frac{m_i \mp m_j}{p^2} [\langle \bar{q}_i q_i \rangle \mp \langle \bar{q}_j q_j \rangle]. \end{aligned} \tag{3.5}$$

This implies the following relations between the Lorentz scalar function of Eqs. (3.3) and (3.5)

$$s^2 \Pi^{V/A,(0)}(p^2) = (m_i \mp m_j) \Pi^{S,P}(p^2) + (m_i \mp m_j)[\langle \bar{q}_i q_i \rangle \mp \langle \bar{q}_j q_j \rangle], \tag{3.6}$$

$$\Pi^{V/A}, (1+0)(p^2) \equiv \Pi^{V/A,(1)}(p^2) + \Pi^{V/A,(0)}(p^2) = \Pi^{V/A}(p^2). \tag{3.7}$$

Consequently, in the chiral limit ($m_i \to 0$) the longitudinal (Spin-0) component, proportional to the quark masses, vanishes. With these definitions one can then derive the inclusive decay ratio:

$$R_\tau = 12\pi S_{EW} \int_0^{m_\tau^2} \frac{\mathrm{d}s}{m_\tau^2} \left(1 - \frac{s}{m_\tau^2} \right)^2 \left[\left(1 + 2\frac{s}{m_\tau^2} \right) \mathrm{Im}\, \Pi^{(T)}(s) + \mathrm{Im}\, \Pi^{(L)}(s) \right], \tag{3.8}$$

[5] As mentioned before, due to it's mass the τ-lepton cannot decay into the heavier quarks top, bottom and charm.

where S_{EW} is an electroweak correction factor.

With the help of the QCD Sum Rules, more specifically the FESR we can then rewrite the tau decay ratio (3.8) into

$$R_\tau = 6\pi i S_{EW} \oint_{|s|=m_\tau^2} \frac{\mathrm{d}s}{m_\tau^2} \left(1 - \frac{s}{m_\tau^2}\right)^2 \left[\left(1 + 2\frac{s}{m_\tau^2}\right) \mathrm{Im}\,\Pi^{(T)}(s) + \mathrm{Im}\,\Pi^{(L)}(s)\right]. \tag{3.9}$$

Normally, using the FESR, we need to pay attention to the integral, which runs along the real axis where the perturbation theory is not valid anymore. This problems close to the real axis are believed to be caused by duality violations. The normal procedure would be to introduce so called pinched weight function, which vanishes at the real axis. However, in the case of the τ-decay ratio we naturally derived a pinched weight function (App. **??**)

$$w_\tau(s) = \left(1 - \frac{s}{m_\tau^2}\right)\left(1 + 2\frac{s}{m_\tau^2}\right), \tag{3.10}$$

which introduce a double zero at $s = m_\tau^2$. The sum rules using pinched weight functions are also referred to as pinched weighted finite energy sum rules or pFESR. It is convenient to rewrite Eq. (**??**) as

$$R_\tau = 6\pi i S_{EW} \oint_{|s|=m_\tau^2} \frac{\mathrm{d}s}{m_\tau^2} \left(1 - \frac{s}{m_\tau^2}\right)^2 \left[\left(1 + 2\frac{s}{m_\tau^2}\right) \mathrm{Im}\,\Pi^{(T+L)}(s) - \left(2\frac{s}{m_\tau^2}\right) \mathrm{Im}\,\Pi^{(L)}(s)\right], \tag{3.11}$$

where we simply reordered the spin composition

$$\Pi^{(T+L)}(s) = \Pi^{(T)}(s) + \Pi^{(L)}(s). \tag{3.12}$$

Unfortunately the two-points functions $\Pi^{(J)}$ are not RG invariant and contains scale and scheme dependent subtractions constants. Noticing that the decay ratio integral (Eq. (**??**)) is RG invariant we can define the so called Adler function, which by itself is RG invariant

$$D^{(L+T)}(s) \equiv -s\frac{\mathrm{d}}{\mathrm{d}s}\left(\Pi^{(L+T)}(s)\right), \quad D^{(L)}(s) = \frac{s}{m_\tau^2}\frac{\mathrm{d}}{\mathrm{d}s}\left(s\Pi^{(L)}(s)\right). \tag{3.13}$$

Making use of integration by parts yields

$$R_\tau = -\pi i \oint_{|s|=m_\tau^2} \frac{\mathrm{d}s}{s} \left(1 - \frac{s}{m_\tau^2}\right)^3 \left[3\left(1 + \frac{s}{m_\tau^2}\right) D^{(L+T)}(s) + 4D^{(L)}(s)\right], \tag{3.14}$$

which can be calculated within QCD.

3.1 The theoretical description of the correlator $\Pi(s)$

3.1.1 The perturbative contribution

We will perform our analysis in the chiral limit, which cancels the longitudinal part of the two point function $\Pi^{(L)}(s) = 0$[6]. This leaves us with with the $\Pi_V^{(T+L)}(s)$ component, which can generally be expressed as [1]

$$\Pi_V^{(T+L)}(s) = -\frac{N_c}{12\pi^2} \sum_{n=0}^{\infty} a_\mu^n \sum_{k=0}^{n+1} c_{nk} L^k, \tag{3.15}$$

[6]The longitudinal part is proportional to the quark masses. Hence zero in the limit of zero quark masses

with

$$L \equiv \log\left(\frac{-s}{\mu}\right) \quad \text{and} \quad a_\mu \equiv a(\mu^2) = \frac{a_s(\mu)}{\pi} \tag{3.16}$$

and μ being the renormalisation scale. With the help of Eq. (3.13) we can rewrite the former expression into terms of the RG invariant Adler function

$$D_V^{(T+L)}(s) = \frac{N_c}{12\pi^2} \sum_{n=0}^{\infty} a_\mu^n \sum_{k=1}^{n+1} k c_{nk} L^{k-1} \tag{3.17}$$

, where the coefficients $c_{n,k}$ are given in App. B.

4 Theory

$\Pi(q^2)$ itself is not a physical quantity. However, we can define two physical quantities out of the two-point correlator. Setting $s = q^2$, the spectral function $\rho(s)$ and the Adler function $D(s)$ are given by

$$\rho(s) \equiv \frac{1}{\pi} Im\Pi(s) \qquad D(s) \equiv -s\frac{d\Pi(s)}{ds} \tag{4.1}$$

Using Kramers-Kronig relation we can connect the theoretical, non physical quantity $\Pi(s)$ with the experimental measurable spectral function $\rho(s)$. With Kramer-Kronic relation we can display the real part of a function as its imaginary part and vice verse. Let $f(x) = Ref(x) + iImf(x)$ be a complex function of the variable s. Suppose this function is analytic in the closed upper half-plane of s and vanishes like $1/|s|$ as $|s| \to \infty$. Then the real part of f can be given as integral over the complex part of f

$$Ref(s) = \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{Imf(s')}{s' - s} ds' \tag{4.2}$$

To derive the Kramers-Kronig relation we start from Cauchy's theorem. Given an analytic function $f(s)$ in the closed upper half plane. The function $s' \to f(s')/(s' - s)$, where s and s' are real values, is also be analytic in the upper half of the plane. The Cauchy's residum theorem then consequently states that

$$\oint \frac{f(s')}{s' - s} ds' = 0. \tag{4.3}$$

include graph Following the contour integral in figure above we are left with

$$\begin{aligned} \oint \frac{f(s')}{s' - s} ds' &= \int_{-R}^{-\epsilon} \frac{f(s')}{s' - s} ds' + \int_{\gamma_{\epsilon^+}} \frac{f(s')}{s' - s} ds' + \int_{\epsilon}^{R} \frac{f(s')}{s' - s} ds' + \int_{\gamma_R}^{+} \frac{f(s')}{s' - s} ds' \\ &= \oint_{-\infty}^{\infty} \frac{f(s')}{s' - s} ds', \end{aligned} \tag{4.4}$$

where the integral along upper semicircle vanishes due to the fact, that in the limit $R \to \infty$ the function $f(s')$ vanishes faster than $1/|s'|$. Furthermore we passed the half-circle to zero. why possible? The real line integral we are left with can be solved using the Sokhotski-Plemelj theorem. Starting by the integral

$$\begin{aligned} \lim_{n \to 0^+} \int_a^b \frac{f(x)}{x + i\epsilon} dx &= \lim_{\epsilon \to 0^+} \int_a^b \frac{x - i\epsilon}{(x + i\epsilon)(x - i\epsilon)} \\ &= -i\pi \lim_{\epsilon \to 0^+} \int_a^b \frac{f(x)}{\pi(x^2 + \epsilon^2)} + \lim_{\epsilon \to 0^+} \int_a^b \frac{x^2}{x^2 + \epsilon^2} \frac{f(x)}{x} dx, \end{aligned} \tag{4.5}$$

where the first term in the second expression is the nasent delta function and therefore approaches a dirac delta function and turns into $-i\pi f(0)$. The second term of the second idendity is approches 1 for $|x| \ll \epsilon$ and 0 for $|x| \gg \epsilon$. Additionally it is totally symmetrix about 0 (which is important for the Cauchy principal value) and turns in the limit into Cauchys principal value integral given by

$$P \int_L f(x) dx = \lim_{\epsilon \to 0} \int_{L(\epsilon)} f(x) dx \tag{4.6}$$

Consequently we get the Sokhotski-Plemelj theorem

$$\lim_{\epsilon\to 0^+}\int_a^b \frac{f(x)}{x-i\epsilon}dx = -i\pi f(x). \tag{4.7}$$

Finally we can we just have to plug in the theorem and change the formula

$$\begin{aligned} 0 &= \oint \frac{f(s')}{s'-s}ds' = P\int_{-\infty}^{\infty}\frac{f(s')}{s'-s} - i\pi f(s) \\ \Rightarrow f(s) &= \frac{P}{i\pi}\int_{-\infty}^{\infty}\frac{f(s')}{s'-s}. \end{aligned} \tag{4.8}$$

Remebering the definition of the spectral function $\rho(s)$ we can now express the two-point correlator $\Pi(s)$ as

$$\Pi(s) = \int_0^{\infty}\frac{\rho(s')}{s'-s-i0}ds' + P(s) \tag{4.9}$$

what happend with the Cauchy principal value (symmetry about 0?), what is P(s) (carries required scale dependence???) think about this once again, at least one more step to ρ function The starting point for a QCD analysis of the e^+e^- scattering is the finite energy sum rule (FESR) cite?

$$\frac{\sigma(e^+e^-\to\gamma^*\to q\bar{q})}{\sigma(e^+e^-\to\mu^+\mu^-)} \equiv R_q(s) = \int_0^{s_0} w(s)\rho(s)ds = -\frac{1}{2\pi i}\oint_{|s|=s_0} w(s)\Pi(s)ds \tag{4.10}$$

how are now 1.15 and 1.16 connected? Why can we write Rq as the integral from 0 to s0 over the w(s) times p(s)? In the massless case the vector correlation function $\Pi(s)$ can be written as follows

$$\Pi(s) = -\frac{N_c}{12\pi^2}\sum_{n=0}^{\infty}a_\mu^n\sum_{k=0}^{n+1}c_{nk}(L)^k, \qquad \text{where} \qquad L\equiv\ln\frac{-s}{\mu^2} \tag{4.11}$$

and $a_\mu = a = \alpha_s/\pi$. Consequently the pertubative expansion of the Adler function $D(s)$ can be writte as

$$D(s) = \frac{N_c}{12\pi^2}\sum_{n=0}^{\infty}a_\mu^n\sum_{k=0}^{n+1}c_{nk}k(L)^{k-1}. \tag{4.12}$$

The spectral function $\rho(s)$ and the Adler function $D(s)$ are physical quantities, so that they have to follow the homogenous renormalisation group equation (RGE)

$$-\mu\frac{d}{d\mu}\begin{Bmatrix}D(s)\\ \rho(s)\end{Bmatrix} = \left[2\frac{\partial}{\partial L}+\beta(a)\frac{\partial}{\partial a}\right]\begin{Bmatrix}D(s)\\ \rho(s)\end{Bmatrix} = 0, \tag{4.13}$$

where we simply used the known form of the homogenous RGE, substitutet $\mu\to L$ and multiplied by -1. The known RGE is given by

$$\left\{\mu\frac{\partial}{\partial\mu}-\beta(a_s)\frac{\partial}{\partial a_s}-\gamma(a_s)m\frac{\partial}{\partial m}\right\}R(q,a_s,m) = 0, \tag{4.14}$$

where $R(q, a_s, m)$ represents an arbitrary physical quantity. In our case these physical quantity is represented by the Adler or the Spectral function. As we neclected the mass the partial derivative of the mass $\partial/\partial m$ vanishes. Furthermore the subsitution is given by

$$L = \ln \frac{-s}{\mu^2} = \ln(-s) - 2\ln(\mu) \qquad \Rightarrow \frac{\partial L}{\partial \mu} = -\frac{2}{\mu}. \tag{4.15}$$

Inserting the substition in eq. 4.14 and multiplying with -1 then yields eq. 4.13.

In the RGE we we have used the β-function, which is defined as

$$-\mu \frac{da}{d\mu} \equiv \beta(a) = \beta_1 a^2 + \beta_2 a^3 + \beta_3 a^4 + \beta_4 a^5 + \cdots \tag{4.16}$$

and known numerically for $N_c = 3$ in the $\bar{M}S$-scheme cite, jamin 27 up to fourth coefficient by cite, jamin 28-30

$$\beta_1 = \frac{11}{2} - \frac{1}{3}N_f, \qquad \beta_2 = \frac{51}{4} - \frac{19}{12}N_f, \qquad \beta_3 = \frac{2857}{64} - \frac{5033}{576}N_f + \frac{325}{1728}N_f^2,$$
$$\beta_4 = \frac{149753}{768} + \frac{891}{32}\zeta_3 - \left(\frac{1078361}{20736} + \frac{1627}{864}\zeta_3\right)N_f + \left(\frac{50065}{20736} + \frac{809}{1296}\zeta_3\right)N_f^2 + \frac{1093}{93312}N_f^3. \tag{4.17}$$

Now we want to have a closer look to the coefficients c_{nk} used in the pertubative expansion of the Adler and the Spectral function. Obviouslu the coefficients c_{n0} have to vanish in both, the Spectral function (it is purely imaginary and the coefficient is real) and the Adler function (it has a factor k), thus the c_{n0} are unphysically and do not appear in measurable quantities. Furthermore the homogenous RGE (eq. **??**) puts constraints on the coefficients c_{nk}. Considering c_{n1} to be independet all other coefficients c_{nk} with $k = 2, \cdots, n+1$ can be expressed with c_{n1} and the β-function up to order α_s^2. Hence the RG contraints lead to

$$c_{22} = -\frac{\beta_1}{4}c_{11}, \qquad c_{33} = \frac{\beta_1^2}{12}c_{11}, \qquad c_{32} = -\frac{1}{4}(\beta_2 c_{11} + 2\beta_1 c_{21}), \tag{4.18}$$
$$c_{44} = -\frac{\beta_1^3}{32}c_{11}, c_{43} = \frac{\beta_1}{24}(5\beta_2 c_{11} + 6\beta_1 c_{21}), c_{42} = -\frac{1}{4}(\beta_3 c_{11} + 2\beta_2 c_{21} + 3\beta_1 c_{31}).$$

Additionally the coefficients, $c_{n,n+1} = 0$ for $n \geq 1$. The independent coefficients c_{n1} are known analytically up to order α_s^3 cite, jamin 31,32 ant at $N_c = 3$ in the $\bar{M}S$-scheme take the following values

$$c_{01} = c_{11} = 1, c_{21} = \frac{365}{24} - 11\zeta_3 - \left(\frac{11}{12} - \frac{2}{3}\zeta_3\right)N_f, \tag{4.19}$$
$$c_{31} = \frac{87029}{288} - \frac{1103}{4}\zeta_3 + \frac{275}{6}\zeta_5 - \left(\frac{7847}{216} = \frac{262}{9}\zeta_3 + \frac{25}{9}\zeta_5\right)N_f + \left(\frac{151}{162} - \frac{19}{27}\zeta_3\right)N_f^2.$$

4.1 Theory equals Experiment

$$\begin{aligned}\int_{C_2} \mathrm{d}s\Pi(s) &= -\int_{C_1} \mathrm{d}s\Pi(s) \\ &= -\int_{0+i\epsilon}^{s_0+i\epsilon} \Pi(s)\,\mathrm{d}s - \int_{0-i\epsilon}^{s_0-i\epsilon} \Pi(s)\,\mathrm{d}s \\ &= -\int_0^{s_0} \Pi(s'+i\epsilon)\,\mathrm{d}s' - \int_0^{s_0} \Pi(s'-i\epsilon)\,\mathrm{d}s' \qquad (4.20) \\ &= -\int_0^{s_0} (\Pi(s'+i\epsilon) - \Pi*(s'+i\epsilon))\,\mathrm{d}s' \\ &= -\int_0^{s_0} 2i\,\mathrm{Im}\,\Pi(s'+i\epsilon)\end{aligned}$$

$$-\int_0^{s_0} 2\,\mathrm{Im}\,\Pi(s)\,\mathrm{d}s = \oint_{|s|=s_0} \Pi(s)\,\mathrm{d}s \qquad (4.21)$$

$$-\int_0^{s_0} \rho_{exp}(s) = -\frac{1}{2\pi i}\oint_{|s|=s_0} \Pi(s)\,\mathrm{d}s \qquad (4.22)$$

4.2 Transform Two Point Function to Adler Function via Complex Contour Integration by Parts

Remember the definition of the **Adler function**:

$$D \equiv -s\frac{\mathrm{d}}{\mathrm{d}s}\Pi(s). \qquad (4.23)$$

Having a look at the **Fundamental theorem of calculus** we can write for a path $\gamma : [0,1] \to \mathbb{C}$

$$\int_\gamma f(z)\,\mathrm{d}z = F(z_1) - F(z_0) \quad \text{or} \quad f(\gamma(1)) - f(\gamma(0)) = \int_\gamma f'(z)\,\mathrm{d}z. \qquad (4.24)$$

Using the definition of the contour integration

$$\int_\gamma f(z)\,\mathrm{d}z = \int_0^1 f(\gamma(t))\gamma'(t)\,\mathrm{d}t = \int_0^1 (f\circ\gamma)'(t)\,\mathrm{d}t \qquad (4.25)$$

the **complex integration by parts** is given by

$$\begin{aligned}\int_\gamma f'(z)g(z)\,\mathrm{d}z &= \int_0^1 f'(\gamma(t))g(\gamma(t))\gamma'(t)\,\mathrm{d}t \\ &= \int_0^1 (f\circ\gamma)'(t)(g\circ\gamma)(t)\,\mathrm{d}t \\ &= [(f\circ\gamma)(t)(g\circ\gamma)(t)]_0^1 - \int_0^1 (f\circ\gamma)(t)(g\circ\gamma)'(t)\,\mathrm{d}t \\ &= -\int_0^1 f(\gamma(t))g'(\gamma(t))\end{aligned} \qquad (4.26)$$

for a closed path (the boundary term vanished for same start and end point). Applying **complex integration by parts** let's us substitute the **Two-Point function** by the **Adler function**

$$\oint_{|s|=s_0} w(s)\Pi(s) = -\oint_{|s|=s_0} \hat{w}(s)\frac{\mathrm{d}\Pi(s)}{\mathrm{d}s} = \oint_{|s|=s_0} \frac{\hat{w}(s)}{s}D(s). \qquad (4.27)$$

4.3 Pearson's χ^2 test

$$\chi^2(\alpha) = [I_i^{exp} - I_i^{th}(\alpha)] C_{ij}^{-1} [I_j^{exp} - I_j^{th}(\alpha)] \tag{4.28}$$

with

$$\begin{aligned} I_i^{exp} &= -\int_0^{s_0} \rho_{exp}(s)\,\mathrm{d}s \\ I_i^{th}(\alpha) &= \oint_{|s|=s_0} \Pi(s)\,\mathrm{d}s \\ C &= \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma 2 & \rho_{13}\sigma_1\sigma_3 & \cdots \\ \rho_{21}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 & \cdots \\ \rho_{31}\sigma_1\sigma 2 & \rho_{32}\sigma_2\sigma_3 & \sigma_3^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{aligned} \tag{4.29}$$

5 Adler function Contributions

$$\beta_1 = \frac{11}{2} - \frac{1}{3}N_f, \quad \beta_2 = \frac{51}{4} - \frac{19}{12}N_f, \quad \beta_3 = \frac{2857}{64} - \frac{5033}{576}N_f + \frac{325}{1728}N_f^2, \tag{5.1}$$

$$\beta_4 = \frac{149753}{768} + \frac{891}{32}\zeta_3 - \left(\frac{1078361}{20736} + \frac{1627}{864}\zeta_3\right)N_f + \left(\frac{50065}{20736} + \frac{809}{1296}\zeta_3\right)N_f^2 + \frac{1093}{93312}N_f^3 \tag{5.2}$$

5.1 Dimension Zero

$$D(s) = \frac{1}{4\pi^2}\sum_{n=0}\tilde{K}_n(\mu)a^n(-\mu s^2) \tag{5.3}$$

$$\tilde{K}_0(\mu) = K_0, \quad \tilde{K}_1(\mu) = K_1, \quad \tilde{K}_2(\mu) = K_2 - \beta_1 K_1 \ln(\mu) \tag{5.4}$$

$$\tilde{K}_3(\mu) = K_3 - [\beta_2 K_1 + 2\beta_1 K_2]\ln\mu + \beta_1^2 K_1 \ln^2\mu \tag{5.5}$$

$$K_0 = K_1 = 1, \quad K_2 = \frac{295}{24} - 9\zeta_3, \quad K_3 = \frac{58057}{288} - \frac{779}{4}\zeta_3 - \frac{75}{2}\zeta_5 \tag{5.6}$$

6 The Experimental Spectral Moments

The general form of the spectral moment can be defined as:

$$I_{exp} = \int_0^{s_0} \frac{ds}{s_0}\omega_\tau\left(\frac{s}{s_0}\right)\rho_{exp}(s). \tag{6.1}$$

This is the experimental side we need to build our χ^2 method to fit our parameters to the data. The spectral-function of the inclusive Hadron τ decays is connected to the total decay rate

$$R_\tau = 12\pi^2\int_0^{s_\tau}\frac{\mathrm{d}s}{s_\tau}\left(1-\frac{s}{s_\tau}\right)^2\left[\left(1+2\frac{s}{s_\tau}\right)\rho_{V+A}^{(1+0)} - 2\frac{s}{s_\tau}\rho_{V+A}^{(0)}(s)\right] \tag{6.2}$$

where $s_\tau = m_\tau^2$ and $\rho^{(1)}(s)$ as well as $\rho^{(0)}(s)$ being the transversal and the longitudinal spectral functions, which are related to the theoretical vector/axialvector (V/A) correlators and implicitly contain the CKM ($|V_{ud}|^2$) and electro-weak (S_{EW}) correction factors.

The total decay rate R is measured within the experiments and is provided by the *Aleph group* as a Fortran subroutine, outputting the binned, normalized invariant mass squared distribution

$$\int_0^{m_\tau^2} \mathrm{d}s\, \mathrm{sfm2}_{V/A}(s) = \int_0^{m_\tau^2} \mathrm{d}s B_i \left(\frac{\mathrm{d}N_i}{N_i\, \mathrm{d}s}\right) \times 100 = B_i \times 100 = R_{\tau,i} B_e \times 100 \tag{6.3}$$

of the non-strange hadronic tau decays for the respective channel i={V-channel, the A-channel, the combined V+A and V-A channels}.

Knowing that the contribution of the longitudinal spectral function is neglect-able[7] we can rewrite the total decay width into

$$R_{\tau,V/A} = 12\pi^2 \int_0^{s_\tau} \frac{\mathrm{d}s}{s_\tau} \left(1 - \frac{s}{s_\tau}\right)^2 \left(1 + 2\frac{s}{s_\tau}\right) \rho_{V+A}^{(1+0)}, \tag{6.4}$$

which we can connect to the binned experimental data

$$\mathrm{sfm2}(sbin) = 100 \times \frac{12\pi^2 B_e}{s_\tau} \underbrace{\int_{sbin-0.5dsbin}^{sbin+0.5dsbin} \mathrm{d}s \left(1 - \frac{s}{s_\tau}\right)^2 \left(1 + s\frac{s}{s_\tau}\right)}_{\omega_\tau} \rho_{exp}(sbin) \tag{6.5}$$

$$= 100 \times \frac{12\pi^2 B_e}{s_\tau} \omega_\tau \rho_{exp}(sbin), \tag{6.6}$$

where *sbin* denotes the denotes the center of the data bin with a given bin width *dsbin*[8]. The needed spectral function is therefore given by:

$$\rho_{exp} = \frac{s_\tau}{100 \times 12\pi^2 B_e \omega_\tau}\, \mathrm{sfm2}(sbin) \tag{6.7}$$

As we related now the data (sfm2) to the spectral function (ρ_{exp}) we can write out the final expression used for the weighted experimental spectral moments

$$I_{exp,\omega} = \sum_{sbin \le s_0} \left(\int_{sbin-0.5dsbin}^{sbin+0.5dsbin} \mathrm{d}s\omega \left(\frac{s}{s_0}\right) \rho_{exp}(sbin) \right) \tag{6.8}$$

$$i\mathcal{M} = (-i)^2 \frac{g^2}{2} \bar{u}(p_\tau)\gamma_\mu \left(\frac{1-\gamma^5}{2}\right) u(p_\nu) \frac{-i}{M_W^2} \left(\frac{i}{4}\frac{g^2}{2}\Pi^{\mu\nu}(q)\right) \times \frac{-i}{M_W^2} \tag{6.9}$$

[7] Apart from the pion-pion pole contribution, which we'll substract from the data.

[8] The bin widths given in the Aleph data are not equidistant, but given

A Derivation of the τ-decay ratio

One of the central formulas of our QCD τ-decay analysis is the τ-decay ratio

$$R_\tau = 12\pi S_{EW} \int_0^{m_\tau^2} \frac{\mathrm{d}s}{m_\tau^2} \left(1 - \frac{s}{m_\tau^2}\right)^2 \left[\left(1 + 2\frac{s}{m_\tau^2}\right) \mathrm{Im}\,\Pi^{(1)}(s) + \mathrm{Im}\,\Pi^{(0)}(s)\right]. \tag{A.1}$$

It was originally derived by Tsai in 1971 [8] and will be probed in the following the guide of [6].

First we need to remember the Lorentz-decomposition of the QCD correlator

$$\Pi_{\mu\nu}(q) = (q_\mu q_\nu - q^2 g_{\mu\nu})\Pi^{(T)}(q^2) + q^\mu q^\nu \Pi^{(L)}(q^2). \tag{A.2}$$

The desired decay-ratio can be expressed as

$$R_\tau = \frac{\Gamma(\tau \to hadrons)}{\Gamma(\tau \to e\nu_\tau \bar{\nu}_e)} \tag{A.3}$$

so we need to make use of the general decay-rate defined as

$$\Gamma = \frac{1}{2M_A} \int \left(\Pi_f \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{1}{2E_f}\right) |\mathcal{M}(A \to \sum_f f)|^2 (2\pi)^4 \delta(p_A - \sum_f p_f), \tag{A.4}$$

where $|\mathcal{M}|^2$ is the squared decay matrix element. As we do not know all the corrections of quark interactions within the τ-decay we want to make use of the optical theorem. The optical theorem states that the before mentioned squared decay matrix element $|\mathcal{M}|^2$, as in Fig. A b), is twice the imaginary part of two times the diagram, like in Fig. A a). Consequently we will calculate the squared decay matrix element of a) in A and use its imaginary part, dividing by a factor of two to get to the needed τ decay rate. Within the τ-decay rate we furthermore have to sum over all possible hadronic final states and integrate over their phase space factors to deal with the momentum-δ, leaving us with an integration over the τ-neutrino.

Starting with the diagrammatical evaluation of Fig. A a), making use of of the Feynman rules, we get

$$\begin{aligned} i\mathcal{M} = (-i)^2 \frac{g^2}{2} \bar{u}(p_\tau)\gamma_\nu \left(\frac{1-\gamma^5}{2}\right) u(p_{\nu_\tau}) \frac{-i}{M_W^2} \left(\frac{i}{4}\frac{g^2}{2}\Pi^{\mu\nu}(q)\right) \\ \times \frac{-i}{M_W^2} \bar{}(p_{\nu_\tau})\gamma_\nu \left(\frac{1-\gamma^5}{2}\right) u(p_\tau). \end{aligned} \tag{A.5}$$

Focusing on the spinors, while summing over the spins we can evaluate the traces

$$\frac{1}{2} \sum_{spins} \bar{u}(p_\tau)\gamma_\mu \left(\frac{1-\gamma^5}{2}\right) u(p_{\nu_\tau}) \bar{u}(p_{\nu_\tau})\gamma_\nu \left(\frac{1-\gamma^5}{2}\right) u(p_\tau) \tag{A.6}$$

$$= \frac{1}{2}\,\mathrm{Tr}\left[\not{p}_\tau \gamma_\mu \left(\frac{1-\gamma^5}{2}\right) \not{p}_{\nu_\tau} \gamma_\nu \left(\frac{1-\gamma^5}{2}\right)\right] \tag{A.7}$$

$$= \frac{1}{2}\,\mathrm{Tr}\left[\not{p}_\tau \gamma_\mu \not{p}_{\nu_\tau} \gamma_\nu \left(\frac{1-\gamma^5}{2}\right)\right] \tag{A.8}$$

$$= (p_\tau^\mu p_{\nu_\tau}^\nu + p_\tau^\nu p_{\nu_\tau}^\mu - g^{\mu\nu} p_{\nu_\tau} \dot{p}_\tau - i\epsilon^{\alpha\mu\beta\nu} p_{\tau,\alpha} p_{\nu_\tau,\beta}), \tag{A.9}$$

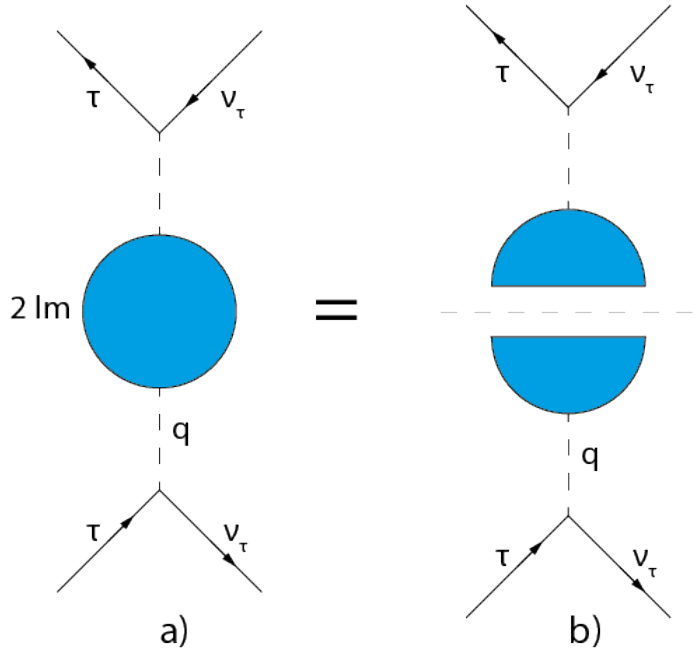

Figure 2. The optical theorem relates the imaginary part of a) to the the hadronic τ decay b). The blue areas, indicate higher order interactions.

which then have to be dotted into (A.5). We notice that $\epsilon^{\alpha\mu\beta\nu}p_{\tau,\alpha}p_{\nu,\beta}$ drops out due to symmetry. We will start regarding only the transversal contribution of the Lorentz-decomposed QCD correlator (A.2) and later infer the missing longitudinal one. Thus we obtain

$$\begin{aligned}\frac{1}{2}\sum_{spins}|\mathcal{M}|^2 &= \frac{g^4}{16M_W^2}(p_\tau^\mu p_\nu^\nu + p_\tau^\nu p_\nu^\mu - g^{\mu\nu}p_\nu p_\tau)(q_\mu q_\nu - q^2 g_{\mu\nu})\Pi^{(T)}(q^2) \\ &= \frac{g^4}{16M_W^2}\left[2(p_\tau\cdot q)(p_\nu\cdot q) + (p_\nu\cdot p_\tau)q^2\right]\Pi^{(T)}(q^2).\end{aligned} \tag{A.10}$$

In the center of mass frame we then can find the needed kinematic expressions

$$2p_\tau\cdot p_\nu = 2p_\nu\cdot q = M_\tau^2 - s \tag{A.11}$$

$$2p_\tau\cdot q = M_\tau^2 + s \tag{A.12}$$

and get the full expression of the transversal amplitude

$$\begin{aligned}&\frac{g^4}{16M_W^2}\frac{1}{2}\left[(M_\tau^2+s)(M_\tau^2-s) + (M_\tau^2-s)s\right]\Pi^{(T)}(q^2) \\ =\ &\frac{g^4}{16M_W^4}\left[\left(1-\frac{s}{M_\tau^2}\right)\left(1+\frac{2s}{M_\tau^2}\right)\right]\mathrm{Im}\,\Pi^{(T)}(q^2).\end{aligned} \tag{A.13}$$

Noting from (A.10) and (A.2) that the longitudinal contribution differs only by a missing

summand $-q^2 g_{\mu\nu}$ we can infer the longitudinal amplitude

$$\begin{aligned} & \frac{g^4}{16M_W^4}(p_\tau^\mu p_\nu^\nu + p_\tau^\nu p_\nu^\mu - g^{\mu\nu} p_\nu p_\tau)(q_\mu q_\nu \Pi^{(L)}(q^2)) \\ = & \frac{g^4}{16M_W^4}[2(p_\tau \cdot q)(p_\nu \cdot q) - (p_\nu \cdot p_\tau)s]\Pi^{(L)}(s) \quad . \\ = & \frac{g^4}{16M_W^4}\left[M_\tau^4\left(1 - \frac{s}{M_\tau}\right)\right]\Pi^{(L)}(s) \end{aligned} \tag{A.14}$$

To get to the inklusive hadron decay we have to deal with the integration

$$\int \frac{\mathrm{d}^3 p_\nu}{(2\pi)^3}\frac{1}{2E_\nu}. \tag{A.15}$$

Due to the massless τ-neutrino and the kinematics we notice that

$$|p_\nu| = \frac{1}{2}\frac{M_\tau^2 - s}{M_\tau} \quad \text{and} \quad E_\nu = p_\nu \tag{A.16}$$

so that the new integrand can be written as: $\mathrm{d}p = -\frac{\mathrm{d}s}{2M_\tau}$. Thus we get a factor of

$$\begin{aligned} \int \frac{\mathrm{d}^3 p_\nu}{(2\pi)^3}\frac{1}{2E_\nu} &= -\int \frac{\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}s}{(2\pi)^3}\frac{1}{2M_\tau}\frac{p_\nu^2}{2p_\nu}\sin^2\theta \\ &= -\int \frac{\mathrm{d}\Omega}{(2\pi)^3}\frac{\mathrm{d}s}{4\dot{2}}\left(\frac{M_\tau^2 - s}{M_\tau^2}\right) \quad . \\ &= \int_0^{M_\tau^2}\frac{4\pi M_\tau^2\,\mathrm{d}s}{(2\pi)^3 8}\left(1 - \frac{s}{M_\tau}\right) \end{aligned} \tag{A.17}$$

for the integration part of the τ-decay rate. Now we just have to combine the longitudinal and transversal contribution with the before evaluated integration factor yielding the final decay rate:

$$\begin{aligned} \Gamma(\tau \to hadrons) = \frac{1}{2M_\tau}\int_0^{M_\tau^2}\frac{g^4 M_\tau^6}{M_\tau^2 2^8 \pi^2 M_W^4}\left(1 - \frac{s}{M_\tau^2}\right)^2 \\ \times\left[\left(1 + 2\frac{s}{M_\tau}\right)\mathrm{Im}\,\Pi^{(T)}(s) + \mathrm{Im}\,\Pi^{(L)}(s)\right]. \end{aligned} \tag{A.18}$$

The τ decay rate into electron-neutrinos is

$$\Gamma(\tau \to e\nu_\tau\bar{\nu}_e) = \frac{G_F^2 M_\tau^5}{192\pi^3} = \frac{g^4 M_\tau^5}{32\dot{1}92 M_W^4 \pi^3}, \tag{A.19}$$

so that the desired ratio is given by

$$R_\tau = 12\pi\int_0^{M_\tau^2}\frac{\mathrm{d}s}{M_\tau^2}\left(1 - \frac{s}{M_\tau^2}\right)\left[(1 + 2\frac{s}{M_\tau^2}\,\mathrm{Im}\,\Pi^{(T)}(s) + \mathrm{Im}\,\Pi^{(L)}(s)\right] \tag{A.20}$$

B Coefficients

Taken from [2]

B.1 β function

$$\beta_1 = \frac{1}{6}(11N_c - 2N_f), \quad \beta_2 = \frac{1}{12}(17N_c^2 - 5N_cN_f - 3C_fN_f),$$
$$\beta_3 = \frac{1}{32}\left(\frac{2857}{54}N_c^3 - \frac{1415}{54}N_c^2N_f + \frac{79}{54}N_cN_f^2 - \frac{205}{18}N_cC_fN_f + \frac{11}{9}C_fN_f^2 + C_f^2N_f\right), \quad \text{(B.1)}$$
$$\beta_4 = \frac{140599}{2304} + \frac{445}{16}\zeta(3),$$

with $C_f = (N_c^2 - 1)/2N_c$.

B.2 γ-function

$$\begin{aligned}
\gamma_1 &= \frac{3}{2}C_f, \quad \gamma_2 = \frac{C_f}{48}(97N_c + 9C_f - 10N_f), \\
\gamma_3 &= \frac{C_f}{32}\left[\frac{11413}{108}N_c^2 - \frac{129}{4}N_cC_f - \left(\frac{278}{27} + 24\zeta(3)\right)N_cN_f + \frac{129}{2}C_f^2\right. \\
&\quad \left. - (23 - 24\zeta(3))\,C_fN_f - \frac{35}{27}N_f^2\right], \\
\gamma_4 &= \frac{2977517}{20736} - \frac{9295}{216}\zeta(3) + \frac{135}{8}\zeta(4) - \frac{125}{6}\zeta(5).
\end{aligned} \quad \text{(B.2)}$$

B.3 Adler function

$$\begin{aligned}
c_{1,1} &= 1, \quad c_{2,1} = \frac{365}{24} - 11\zeta_3 - \left(\frac{11}{12} - \frac{2}{3}\zeta(3)\right)N_f = 1.640, \\
c_{3,1} &= \frac{87029}{288} - \frac{1103}{4}\zeta_3 + \frac{275}{6}\zeta_5 \\
&\quad - \left(\frac{7847}{216} - \frac{262}{9}\zeta_3 + \frac{25}{9}\zeta_5\right)N_f + \left(\frac{151}{162} - \frac{19}{27}\zeta_3\right)N_f^2 = 6.371, \\
c_{4,1} &= \frac{78631453}{20736} - \frac{1704247}{432}\zeta_3 + \frac{4185}{8}\zeta_3^2 + \frac{34165}{96}\zeta_5 - \frac{1995}{16}\zeta_7 = 49.076
\end{aligned} \quad \text{(B.3)}$$

from [3]

$$\begin{aligned}
c_{2,2} &= \frac{\beta_1 c_{1,1}}{4}, \quad c_{2,3} = 0 \\
c_{3,2} &= -\frac{1}{4}(\beta_2 \quad c_{33} = \frac{\beta_1^2}{12}c_{1,1}, c_{11} + 2\beta_1 c_{2,1}), \quad c_{3,4} = 0 \\
c_{4,2} &= -\frac{1}{4}(\beta c_{11} + 2\beta_2 c_{21} + 3\beta_1 c_{31}), \\
c_{4,3} &= \frac{1}{24}(6c_{2,1}\beta_1^2 + 5\beta_2\beta_1 c_{1,1}), c_{4,4} = -\frac{1}{32}\beta_1^3 c_{1,1}, \\
c_{5,2} &= \frac{1}{4}(-\beta_4 c_{1,1} - 2\beta_3 c_{2,1} - 3\beta_2 c_{3,1} - 4\beta_1 c_{4,1}), \\
c_{5,3} &= \frac{1}{24}(12c_{3,1}\beta_1^2 + 6\beta_1\beta_3 c_{1,1} + 14\beta_2\beta_1 c_{2,1} + 3\beta_2^2 c_{1,1}), \\
c_{5,4} &= \frac{1}{96}(-12\beta_1^3 c_{2,1} - 13\beta_2\beta_1^2 c_{1,1}), c_{5,5} = \frac{1}{80}\beta_1^4 c_{1,1}.
\end{aligned} \quad \text{(B.4)}$$

C Numerical Analysis

[7] [5]

C.1 Finding Roots: Newton-Raphson Method

With the running of the strong coupling α_s we had to solve a non-linear equation. A common method to deal with this problem is rewriting an equation in the form

$$f(x) = 0. \tag{C.1}$$

So we solve for x by finding the root of $f(x)$.

The standard method of numerically solving for the root is called **Newton-Raphson method**. It is an *open method*, meaning that we do not have to *bracket* the root within a before known interval, but rather can start with any x_i and the method will most probably find the position[9] of the root.

Starting by a point x_i we can calculate the tangent, the slope $f'(x_i)$, which root $0 = f'(x_i)$ can be used to generate an iterative description of finding $f(x_r)$, where x_r would be the true root of $f(x)$.

Geometrically we can calculate the root iteratively from the tangent (slope) at $f(x_i)$ as

$$0 = f'(x_i) = \frac{f(x_i)}{x_{i+1} - x_i} \tag{C.2}$$

yielding the Newton-Raphson method

$$x_{i+1} = x_i + \frac{f(x_i)}{f'(x_i)}. \tag{C.3}$$

Another way of deriving the method is by Taylor expanding $f(x_{i+1})$ at x_i up to the second order, which also yield an estimate of the array per iteration i

$$0 \overset{!}{=} f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \mathcal{O}(x_i^2) \quad \Rightarrow \quad x_{i+1} = x_i + \frac{f(x_i)}{f'(x_i)}. \tag{C.4}$$

Then we can take the same Taylor expansion to the 3rd order and obtain an estimate for the Error

$$E_i = x_r - x_i \tag{C.5}$$

for E_{i+1}, while x_r is still the true root for $f(x)$.

$$0 = f(x_i) + f'(x_i)(x_r - x_i) + \frac{f''(x_i)}{2!}(x_r - x_i)^2 + \mathcal{O}(x_i^3) \tag{C.6}$$

including (C.2) yields

$$- f'(x_i)(x_{i+1} - x_i) + f'(x_i)(x_r - x_i) + \frac{f''(x_i)}{2!}(x_r - x_i)^2, \tag{C.7}$$

which then can be rewritten in the form of our iterative error estimator

$$E_{i+1} = x_r - x_{i+1} = \frac{f''(x_i)}{2f'(x_i)}(x_r - x_i)^2 \tag{C.8}$$

[9] In this thesis we only had to deal with singular roots, for multiple roots one should modify the algorithm.

or

$$E_{i+1} = \frac{f''(x_i)}{2f'(x_i)} E_i^2. \tag{C.9}$$

So roughly speaking the error of an iterative step is proportional to the square of the error of the previous error and the result will get up to two digits more accurate with every iteration. As we aim for double precision, meaning 10^-15 we have perform 8 iterations for every root we want to find.

C.2 Newton-Cotes

C.3 Gauss Quadrature

C.4 Runge-Kutta Methods (Ordinary Differential Equations)

Following [**?**] we want to describe a numerical procedure of evaluating ordinary differential equations (ODE) of the form

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y). \tag{C.10}$$

In general we will start with a given point $(x_i|y_i)$ and want to obtain y_{i+1} at a given x_{i+1}[10]. The methods used to solve an ODE numerically can be summed up as **Runge-Kutta methods** and are based on **Euler's method**, which basically takes the slope at the starting point x_i to calculate the function value at the next step y_{i+1}

$$y_{i+1} = y_i + \underbrace{\Phi}_{\text{Slope}} \underbrace{h}_{\text{Step size}}. \tag{C.11}$$

C.4.1 Euler's Method

Euler's method is expressed by

$$y_{i+1} = y_i + f(x_i, y_i)h, \tag{C.12}$$

with $f(x_i, y_i)$ being the slope at x_i and h being the step size ($h = x_{i+1} - x_i$). The method is also refered to as *Euler-Cauchy* or *point-slope* method. Euler's method is approximating the changing slope in the interval h to the slope at the point (x_i) to calculate the function value at x_{i+1}. Having a look at the Taylor-expansion

$$y_{i+1} = y_i + y_i'h + \frac{y_i''}{2!}h^2 + \cdots + \frac{y_i^{(n)}}{n!}h^n + R_n, \tag{C.13}$$

where $h = x_{i+1} - x_i$ and R_n being the remainder term

$$R_n = \frac{y^{(n_1)}(\Psi)}{n+1)!}h^{n+1} \tag{C.14}$$

, where Ψ lies somewhere in the interval from x_i to x_{i+1}. By comparing the Taylor expansion with Euler's method (C.12) on can see that Euler's method represents a first order Taylor expansion, but misses all higher order terms. This higher order terms contribute to a *local error*. Having then more than one step h this local errors then will propagate and form a so called *globalerror*. To improve the global error one has to either perform more steps or include higher order terms of the Taylor expansion.

[10] For our purposes we had to solve the differential equation of the running strong coupling α_s to obtain the different values at different energies. The ODE we solved numerically is given by $\beta(a_s) = -\mu\, \mathrm{d}a_s/\,\mathrm{d}\mu$.

C.4.2 Heun's Method

The main error source of Euler's method is that the derivative at the beginning of the interval is assumed to to apply across the entire step size. To improve this behavior we can use Euler's method in the first step to calculate a so called **predictor** y^0_{i+1} and then average over the slope of the predictor and the starting point, yielding the so called **corrector**

$$\text{Predictor:} \qquad y^0_{i+1} = y_i + f(x_i, y_i)h \tag{C.15}$$

$$\text{Corrector:} \qquad y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1}}{2}h. \tag{C.16}$$

Another advantage of Heun's method is, that one can iteratively can achieve a better result for each step, while averaging multiple times over the "corrected" y-end-point value. At this point one also should notice the similarity between Heun's method and the trapezoidal rule missing integration part we introduced in the context of numerical integration.

C.4.3 Runge-Kutta Methods

The former methods can be summed up within the so called **Runge-Kutta methods**, which basic formula is given by

$$y_{i+1} = y_i + \Phi(x_i, y_i, h)h, \tag{C.17}$$

where $\Phi(x_i, y_i, h)$ is called an *increment function*, which can be interpreted as an representative slope over the interval. The increment function can be written as

$$\Phi = a_1k_1 + a_2k_2 + \cdots + a_nk_n, \tag{C.18}$$

where the a_i's are constants and the k's are defined as

$$k_1 = f(x_i, y_i) \tag{C.19}$$

$$k_2 = f(x_i + p_1h, y_i + q_{11}k_1h) \tag{C.20}$$

$$k_3 = f(x_i + p_2h, y_i + q_{21}k_1h + q_{22}k_2h) \tag{C.21}$$

$$\vdots \tag{C.22}$$

$$k_n = f(x_i + p_{n-1}h, y_i + q_{n-1,1}k_1h + q_{n-1,2}k_2h + \cdots + q_{n-1,n-1}k_{n-1}h), \tag{C.23}$$

where the q's and p's are constant, which have to be determined by comparison of the Taylor expansion of y_{i+1}. The Runge-Kutta methods are given in different orders determined by the biggest subscript of the included k's (e.g. if Φ only depends on k_1 and k_2, the Range-Kutta method will be of second order). As mentioned before we have now several degrees of freedom (a's, q's and p's), which can mostly be fixed from comparison with the Taylor expansion of y_i. The leftover variable can then be freely chosen.

For a second order Runge-Kutta method we can fix all but one variable

$$a_1 = 1 - a_2 \tag{C.24}$$

$$p_1 = q_{11} = \frac{1}{2a_2}. \tag{C.25}$$

For the leftover variabel are three comon selections,

- Heuns method with a single corrector for choosing $a_2 = 1/2$
- the Midpoint method for choosing $a_2 = 1$
- and Ralston's method for choosing $a_2 = 2/3$.

The third order Runge-Kutta method can be shown to take the form

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h \tag{C.26}$$

and the from us implemented forth order Runge-Kutta method is given by

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h, \tag{C.27}$$

with

$$k_1 = f(x_i, y_i) \tag{C.28}$$

$$k_2 = f\left(x_1 + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \tag{C.29}$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right) \tag{C.30}$$

$$k_4 = f(x_i + h, y_i + k_3 h). \tag{C.31}$$

[11]

C.5 Discrepancies between Matthias and my Code

- My spectral moments are slightly lower than Matthias ones (of order 10^{-2}). Could be caused by the different treatment of weight functions. Mine are integrated with Gaussian Quadratures. Matthias are taken at the center and multiplicated with the bin witdth.

[11] The fourth-order Runge-Kutta methods reminds us at the Simpson rule from the numerical integration procedures.

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