hhtop

v1.0

`hhtop` is a tool to compute, numerically, the following quantities for the Haldane-Hubbard model:

- the one-loop renormalization of the topological phase diagram,
- the difference of the (a, a) and (b, b) wave-function renormalizations, at second order,

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1. Phase diagram

In this section we discuss the computation of the renormalization of the phase diagram.

1.1. Description of the computation

1.1.1. Definition of the problem

We wish to solve the following equation:

$$\tilde{M}_{\omega,t_1,t_2,\lambda}(W,\phi) := W + 3\sqrt{3}\omega t_2 \sin\phi + \frac{3\sqrt{3}}{16\pi^3}\lambda \int_{\mathcal{B}} dk \int_{-\infty}^{\infty} dk_0\ \frac{m_{t_2,W,\phi}(k)}{D_{t_1,t_2,W,\phi}(k_0,k)} = 0 \tag{1.1}$$

for $W \in \mathbb{R}$, $\phi \in (-\pi,\pi]$, where the parameters $\omega = \pm 1$, $t_2 \geqslant 0$, $t_1 \geqslant 3t_2$ and $\lambda \in \mathbb{R}$ are fixed. We now define the quantities appearing in (1.1):

$$\mathcal{B} := \left\{ \left(\frac{2\pi}{3} + k_1', k_2\right) \in \mathbb{R}^2 \quad | \quad |k_2| < \frac{2\pi}{\sqrt{3}} - \sqrt{3}|k_1'| \right\}, \tag{1.2}$$

$$\alpha_1(k_1,k_2) := \frac{3}{2} + \cos(\sqrt{3}k_2) + 2\cos\left(\frac{3}{2}k_1\right)\cos\left(\frac{\sqrt{3}}{2}k_2\right), \tag{1.3}$$

$$\alpha_2(k_1,k_2) := -\sin(\sqrt{3}k_2) + 2\cos\left(\frac{3}{2}k_1\right)\sin\left(\frac{\sqrt{3}}{2}k_2\right), \tag{1.4}$$

$$\Omega(k_1,k_2) := 1 + 2e^{-\frac{3}{2}ik_1}\cos\left(\frac{\sqrt{3}}{2}k_2\right), \tag{1.5}$$

$$m_{t_2,W,\phi}(k) := W - 2t_2\sin\phi\,\alpha_2(k) \tag{1.6}$$

$$\zeta_{t_2,\phi}(k) := 2t_2\cos\phi\,\alpha_1(k), \quad \xi_{t_1,t_2,W,\phi}(k) := \sqrt{m^2_{t_2,W,\phi}(k) + t_1^2|\Omega(k)|^2} \tag{1.7}$$

$$D_{t_1,t_2,W,\phi}(k_0,k) := (ik_0 + \zeta_{t_2,\phi}(k))^2 - \xi^2_{t_1,t_2,W,\phi}(k). \tag{1.8}$$

1.1.2. Integration of the Matsubara momentum

We first integrate out k_0 analytically. We use the following identity: for $x \in \mathbb{R}$ and $y > 0$,

$$\int_{-\infty}^{\infty} dk_0\ \frac{1}{((ik_0 + x)^2 - y^2)} = -\chi(x^2 < y^2)\frac{\pi}{y} \tag{1.9}$$

in which $\chi(x^2 < y^2) \in \{1,0\}$ is equal to 1 if and only if $x^2 < y^2$. Furthermore (see appendix (A1)), if

$$t_1 \geqslant 3t_2 \tag{1.10}$$

then

$$\zeta^2_{t_2,\phi}(k) \leqslant \xi^2_{t_1,t_2,W,\phi}(k) \tag{1.11}$$

for all $k \in \mathcal{B}$, $\phi \in (-\pi,\pi]$ and $W \in \mathbb{R}$, which implies that

$$\tilde{M}_{\omega,t_1,t_2,\lambda}(W,\phi) = W + 3\sqrt{3}\omega t_2 \sin\phi - \frac{3\sqrt{3}}{16\pi^2}\lambda \int_{\mathcal{B}} dk\ \frac{m_{t_2,W,\phi}(k)}{\xi_{t_1,t_2,W,\phi}(k)}. \tag{1.12}$$

1.1.3. Reduction by symmetries

By using some symmetries of the integrand of (1.12), we can reduce the integration region. Indeed, $m_{t_2,W,\phi}(k)$ and $\xi_{t_1,t_2,W,\phi}(k)$ are symmetric under $k_1 \mapsto -k_1$ and under rotations of angle $\frac{2\pi}{3}$. In addition, $m_{t_2,W,\phi}(k_1,k_2) = m_{t_2,W,-\phi}(k_1,-k_2)$ and $\xi_{t_1,t_2,W,\phi}(k_1,k_2) = \xi_{t_1,t_2,W,-\phi}(k_1,-k_2)$. We can therefore rewrite

$$\tilde{M}_{\omega,t_1,t_2,\lambda}(W,\phi) = W + 3\sqrt{3}\omega t_2 \sin\phi - \lambda(I_{t_1,t_2}(W,\phi) + I_{t_1,t_2}(W,-\phi)) \tag{1.13}$$

where

$$I_{t_1,t_2}(W,\phi) := \frac{9\sqrt{3}}{8\pi^2}\int_{\mathcal{B}_+} dk\ \frac{m_{t_2,W,\phi}(k)}{\xi_{t_1,t_2,W,\phi}(k)}. \tag{1.14}$$

with

$$\mathcal{B}_+ := \left\{(k_1,k_2)\in\mathcal{B}\ |\ k_2>0,\ k_1<\frac{2}{3}\pi,\ k_2<\frac{1}{\sqrt{3}}k_1\right\}. \tag{1.15}$$

1.1.4. Polar coordinates

Let

$$p_F^{\pm} := \left(\frac{2\pi}{3},\ \frac{2\pi}{3\sqrt{3}}\right). \tag{1.16}$$

We note that $\xi_{t_1,t_2,W,\phi}$ has roots if and only if $m_{t_2,W,\phi}(p_F^+) = 0$ or $m_{t_2,W,\phi}(p_F^-) = 0$, located at p_F^+ in the former case and at p_F^- in the latter. If $m_{t_2,W,\phi}$ vanishes at both $p_F^{\pm}$, which can only occur if $W = 0$ and $\phi = 0,\pi$, then $\xi_{t_1,t_2,W,\phi}$ vanishes at both $p_F^{\pm}$. Nevertheless, the integrand in (1.14) is not singular, since $\xi_{t_1,t_2,W,\phi}(k'+p_F^+) \sim t_1|k'|$, and the integration over k is 2-dimensional. In order to make this lack of singularity apparent, it is convenient to switch to polar coordinates around p_F^+: $(k_1,k_2) = p_F^+ + \frac{2\pi}{3\sqrt{3}}\rho(\cos\theta,\sin\theta)$:

$$I_{t_1,t_2}(W,\phi) = \frac{\sqrt{3}}{6}\int_{-\frac{\pi}{6}}^{\frac{\pi}{6}} d\theta \int_0^{R(\theta)} d\rho\ \rho\frac{\bar{m}_{t_2,W,\phi}(\rho,\theta)}{\bar{\xi}_{t_1,t_2,W,\phi}(\rho,\theta)}, \tag{1.17}$$

in which

$$\begin{gathered}
\bar{m}_{t_2,W,\phi}(\rho,\theta) := W - 2t_2\sin\phi\bar{\alpha}_2(\rho,\theta), \quad \bar{\xi}_{t_1,t_2,W,\phi}(\rho,\theta) := \sqrt{m^2_{t_2,W,\phi}(\rho,\theta) + t_1^2|\bar{\Omega}(\rho,\theta)|^2} \\
\bar{\alpha}_2(\rho,\theta) := -2\sin\left(\tfrac{\pi}{3}(1+\rho\sin\theta)\right)\left(\cos\left(\tfrac{\pi}{3}(1+\rho\sin\theta)\right) + \cos\left(\tfrac{\pi}{\sqrt{3}}\rho\cos\theta\right)\right) \\
|\bar{\Omega}(\rho,\theta)|^2 = 1 + 4\cos\left(\tfrac{\pi}{3}(1+\rho\sin\theta)\right)\left(\cos\left(\tfrac{\pi}{3}(1+\rho\sin\theta)\right) - \cos\left(\tfrac{\pi}{\sqrt{3}}\rho\cos\theta\right)\right)
\end{gathered} \tag{1.18}$$

and

$$R(\theta) := \frac{1}{\cos(\theta - \frac{\pi}{6})}. \tag{1.19}$$

1.2. Strategy of the numerical computation

1.2.1. Newton scheme

In order to solve (1.1), we will use a Newton scheme (see section 3.1). More precisely, we fix ϕ and compute $W(\phi)$ as the limit of

$$\begin{aligned} W_0(\phi) &:= -\omega 3\sqrt{3} t_2 \sin\phi \\ W_{n+1}(\phi) &:= W_n(\phi) - \frac{\tilde{M}_{\omega,t_1,t_2,\lambda}(W_n(\phi),\phi)}{\partial_W \tilde{M}_{\omega,t_1,t_2,\lambda}(W_n(\phi),\phi)}. \end{aligned} \tag{1.20}$$

The first two derivatives of $\tilde{M}$ are

$$\partial_W \tilde{M}_{\omega,t_1,t_2,\lambda}(W,\phi) = 1 - \lambda(\partial_W I_{t_1,t_2}(W,\phi) + \partial_W I_{t_1,t_2}(W,-\phi)) \tag{1.21}$$

with

$$\partial_W I_{t_1,t_2}(W,\phi) = \frac{\sqrt{3}}{6}\int_{-\frac{\pi}{6}}^{\frac{\pi}{6}} d\theta \int_0^{R(\theta)} d\rho\ \frac{\rho}{\bar{\xi}_{t_1,t_2,W,\phi}(\rho,\theta)}\left(1 - \frac{\bar{m}^2_{t_2,W,\phi}(\rho,\theta)}{\bar{\xi}^2_{t_1,t_2,W,\phi}(\rho,\theta)}\right) \tag{1.22}$$

and

$$\partial_W^2 \tilde{M}_{\omega,t_1,t_2,\lambda}(W,\phi) = -\lambda(\partial_W^2 I_{t_1,t_2}(W,\phi) + \partial_W^2 I_{t_1,t_2}(W,-\phi)) \tag{1.23}$$

with

$$\partial_W^2 I_{t_1,t_2}(W,\phi) = -\frac{\sqrt{3}}{2}\int_{-\frac{\pi}{6}}^{\frac{\pi}{6}} d\theta \int_0^{R(\theta)} d\rho\ \frac{\rho \bar{m}_{t_2,W,\phi}(\rho,\theta)}{\bar{\xi}^3_{t_1,t_2,W,\phi}(\rho,\theta)}\left(1 - \frac{\bar{m}^2_{t_2,W,\phi}(\rho,\theta)}{\bar{\xi}^2_{t_1,t_2,W,\phi}(\rho,\theta)}\right). \tag{1.24}$$

1.2.2. Integration

In order to compute $W_n(\phi)$, we have to evaluate $I_{t_1,t_2}(W,\phi)$ and $\partial_W I_{t_1,t_2}(W,\phi)$. The integrations are carried out using Gauss-Legendre quadratures (see section 3.2). In order to use this method to compute the double integral over θ and ρ, we rewrite

$$\int d\theta \int d\rho\ F(\theta,\rho) = \int d\theta\ G(\theta), \quad G(\theta) := \int d\rho\ F(\theta,\rho) \tag{1.25}$$

for the appropriate F.

1.3. Usage and examples

We will now describe some basic usage cases of `hhtop phase`. For a full description of the options of `hhtop`, see the `man` page.

1.3.1. Basic usage

The value of the parameters can be set via the `-p` flag. Here is an example

```
hhtop phase -p "omega=1;t1=1.;t2=.1;lambda=.01;sinphi=1;"
```

Note that ϕ can be set instead of $\sin\phi$, though the result of the computation only depends on $\sin\phi$. The parameters that are not specified by the `-p` flag are set to their default value: $\omega = 1$, $t_1 = 1$, $t_2 = 0.1$, $\lambda = 0.01$, $\sin\phi = 1$.

1.3.2. Precision of the computation

The precision of the computation can be controlled by three parameters: the precision of the numbers manipulated by `hhtop` (set via the `-P` flag, see section 3.3), the order of the integration, and the tolerance of the Newton scheme.

1 - Order of the integration. The order of the integration, that is, the value of the number N introduced in section 3.2, can be specified via the `-O` flag. Its default value is 10. The difference of the value of the integral at different orders is a good measure of the numerical error. Example:

```
hhtop phase -O 30
```

2 - Tolerance of the Newton scheme. The Newton iteration halts when the difference $|x_{n+1} - x_n|$ (see section 3.1) is smaller than a number, called the *tolerance* of the algorithm, or when the toal number of steps exceeds a given threshold. The tolerance can be set via the `-t` flag, and the maximal number of steps via the `-N` flag. Their default values are 10^{-11} and 1000000. The tolerance and maximal number of steps are also used in the computation of the roots $\{x_1, \cdots, x_N\}$ of the N-th Legendre polynomial which are used for the numerical integration (see section 3.2). If the tolerance or the maximal number of steps are too small, and the precision of multi-precision floats is too low, then the iteration may not converge. Example:

```
hhtop phase -t 1e-30 -N 2000000 -O 100 -P 256
```

1.3.3. Using double precision floats instead of multi-precision floats

Using the `-D` command-line flag, `hhtop` can be instructed to use `long double`'s instead of MPFR floats. Whereas one then loses the ability of adjusting the precision, the computation time can be drastically reduced. Example:

```
hhtop -D phase -p "sinphi=1.;"
```

The precision of `long doubles` is compiler dependent, see section 3.3.

2. Wave function renormalization

In this section we discuss the computation of the difference and the sum of the (a, a) and (b, b) wave-function renormalizations.

Warning: This computation is only accurate if ϕ is not too close to 0.

2.1. Description of the computation

2.1.1. Definition of the problem

We wish to compute the following quantities:

$$\begin{aligned} z_1 - z_2 &= i\frac{27}{128\pi^4}(\partial_{k_0}S_+|_{k_0=0} - \partial_{k_0}S_-|_{k_0=0}) \\ z_1 + z_2 &= i\frac{27}{128\pi^4}(\partial_{k_0}S_+|_{k_0=0} + \partial_{k_0}S_-|_{k_0=0}) \end{aligned} \tag{2.1}$$

where

$$S_\pm(k_0) = \int_{\mathcal{B}} dpdq \int_{-\infty}^{\infty} \frac{dp_0dq_0}{2\pi^2}\; \frac{(-ip_0 - \zeta_p \mp m_p)(-iq_0 - \zeta_q \mp m_q)(-i(p_0+q_0-k_0) - \zeta_F \mp m_F)}{((ip_0+\zeta_p)^2 - \xi_p^2)((iq_0+\zeta_q)^2 - \xi_q^2)((i(p_0+q_0-k_0)+\zeta_F)^2 - \xi_F^2)} \tag{2.2}$$

in which

$$\mathcal{B} := \left\{ \left(\frac{2\pi}{3} + k_1', k_2\right) \in \mathbb{R}^2 \quad | \quad |k_2| < \frac{2\pi}{\sqrt{3}} - \sqrt{3}|k_1'| \right\}, \tag{2.3}$$

$$\alpha_1(k_1, k_2) := 2\cos\left(\frac{\sqrt{3}}{2}k_2\right)\left(\cos\left(\frac{3}{2}k_1\right) + \cos\left(\frac{\sqrt{3}}{2}k_2\right)\right) + \frac{1}{2}, \tag{2.4}$$

$$\alpha_2(k_1, k_2) := 2\sin\left(\frac{\sqrt{3}}{2}k_2\right)\left(\cos\left(\frac{3}{2}k_1\right) - \cos\left(\frac{\sqrt{3}}{2}k_2\right)\right), \tag{2.5}$$

$$m(k) := W - 2t_2\sin\phi\,\alpha_2(k) \tag{2.6}$$

$$\zeta(k) := 2t_2\cos\phi\,\alpha_1(k), \quad \xi(k) := \sqrt{m^2(k) + 2t_1^2\alpha_1(k)} \tag{2.7}$$

and

$$\begin{gathered} \zeta_p \equiv \zeta(p), \quad \zeta_q \equiv \zeta(q), \quad \zeta_F \equiv \zeta(p+q-p_F^\omega), \quad \xi_p \equiv \xi(p), \quad \xi_q \equiv \xi(q), \quad \xi_F \equiv \xi(p+q-p_F^\omega), \\ m_p \equiv m(p), \quad m_q \equiv m(q), \quad m_F \equiv m(p+q-p_F^\omega) \end{gathered} \tag{2.8}$$

with $\omega \in \{-1, +1\}$ and

$$p_F^\pm := \left(\frac{2\pi}{3}, \pm\frac{2\pi}{3\sqrt{3}}\right). \tag{2.9}$$

2.1.2. Integration of the Matsubara momentum

We first integrate out p_0 and q_0 analytically. We recall (see appendix (A1)) that, provided $t_1 \geqslant 3t_2$,

$$\zeta^2(k) \leqslant \xi^2(k). \tag{2.10}$$

By closing the integration path over p_0 around the positive-imaginary half-plane (which, by (2.10), contains two poles), and using the residues theorem, we find that

$$\begin{aligned} S_\pm(k_0) = -\int_{\mathcal{B}} dpdq \int_{-\infty}^{\infty} \frac{dq_0}{2\pi} \Bigg(& \frac{(\xi_p \mp m_p)(-iq_0 - \zeta_q \mp m_q)(-i(q_0 - k_0) + \zeta_p - \zeta_F + \xi_p \mp m_F)}{\xi_p((iq_0 + \zeta_q)^2 - \xi_q^2)((i(q_0 - k_0) - \zeta_p + \zeta_F - \xi_p)^2 - \xi_F^2)} \\ & + \frac{(i(q_0 - k_0) - \zeta_p + \zeta_F + \xi_F \mp m_p)(-iq_0 - \zeta_q \mp m_q)(\xi_F \mp m_F)}{((-i(q_0 - k_0) + \zeta_p - \zeta_F - \xi_F)^2 - \xi_p^2)((iq_0 + \zeta_q)^2 - \xi_q^2)\xi_F} \Bigg). \end{aligned} \tag{2.11}$$

We then close the integration path over q_0 around the positive-imaginary half-plane for the first term, and the negative imaginary half-plane for the second, and find

$$\begin{aligned} S_\pm(k_0) = \frac{1}{2} \int_{\mathcal{B}} dpdq \Bigg(& \frac{(\xi_p \mp m_p)(\xi_q \mp m_q)(ik_0 + Z + \xi_p + \xi_q \mp m_F)}{\xi_p \xi_q((ik_0 + Z + \xi_p + \xi_q)^2 - \xi_F^2)} \\ & + \frac{(\xi_q \pm m_q)(\xi_F \mp m_F)(ik_0 + Z - \xi_q - \xi_F \pm m_p)}{\xi_q \xi_F((ik_0 + Z - \xi_q - \xi_F)^2 - \xi_p^2)} \\ & - \frac{(\xi_p \mp m_p)(\xi_F \mp m_F)(ik_0 + Z + \xi_p - \xi_F \pm m_q)}{\xi_p \xi_F((ik_0 + Z + \xi_p - \xi_F)^2 - \xi_q^2)} \Bigg) \end{aligned} \tag{2.12}$$

with

$$Z := \zeta_p + \zeta_q - \zeta_F. \tag{2.13}$$

The sum of the three terms in the right side of (2.12) yields

$$\begin{aligned} S_\pm(k_0) = \frac{1}{2} \int_{\mathcal{B}} dpdq \Bigg(& \frac{(\xi_p\xi_q\xi_F - (\xi_p m_q + \xi_q m_p)m_F + m_p m_q \xi_F)(ik_0 + Z)}{\xi_p\xi_q\xi_F((ik_0 + Z)^2 - (\xi_p + \xi_q + \xi_F)^2)} \\ & \pm \frac{(\xi_p + \xi_q + \xi_F)(m_p\xi_q\xi_F + \xi_p m_q \xi_F - \xi_p\xi_q m_F - m_p m_q m_F)}{\xi_p\xi_q\xi_F((ik_0 + Z)^2 - (\xi_p + \xi_q + \xi_F)^2)} \Bigg). \end{aligned} \tag{2.14}$$

Therefore,

$$\begin{aligned} z_1 - z_2 &= \frac{27}{64\pi^4} \int_{\mathcal{B}} dpdq \left(\frac{(\xi_p + \xi_q + \xi_F)(\frac{m_p}{\xi_p} + \frac{m_q}{\xi_q} - \frac{m_F}{\xi_F} - \frac{m_p m_q m_F}{\xi_p \xi_q \xi_F})Z}{(Z^2 - (\xi_p + \xi_q + \xi_F)^2)^2} \right). \\ z_1 + z_2 &= \frac{27}{128\pi^4} \int_{\mathcal{B}} dpdq \left(\frac{\left(1 - \frac{m_p m_F}{\xi_p \xi_F} - \frac{m_q m_F}{\xi_q \xi_F} + \frac{m_p m_q}{\xi_p \xi_q}\right)(Z^2 + (\xi_p + \xi_q + \xi_F)^2)}{(Z^2 - (\xi_p + \xi_q + \xi_F)^2)^2} \right). \end{aligned} \tag{2.15}$$

2.1.3. Singularities of the integrand

In order to compute the integrals in (2.15) numerically, we will use Gauss quadratures, which are only accurate if the integrands are smooth (i.e. if high order derivatives of the integrand are bounded). In this case, the integrand has singularities, indeed

- α_1 and ζ vanish at p_F^+ and p_F^-, and if $W = -\omega 3\sqrt{3} t_2 \sin\phi$, then m vanishes at p_F^ω,
- if $W = -\omega 3\sqrt{3} t_2 \sin\phi$, then the second derivative of ξ diverges at p_F^ω.

The asymptotics near the singularities are

$$\begin{aligned}\sqrt{2t_1^2\alpha_1(p_F^\omega+k')} &= \frac{3}{2}t_1|k'|+t_1\ O(|k'|^2)\\ \zeta(p_F^\omega+k') &= t_2\cos\phi\ O(|k'|^2)\\ m(p_F^\omega+k')-(W-\omega3\sqrt{3}t_2\sin\phi) &= t_2\sin\phi\ O(|k'|^2)\end{aligned} \tag{2.16}$$

which implies that, if $W=-\omega3\sqrt{3}t_2\sin\phi$, $p=p_F^\omega+p'$, $q=p_F^\omega+q'$ and $k=p_F^\omega$, then

$$\begin{gathered}\xi_p+\xi_q+\xi_F=\frac{3}{2}t_1(|p'|+|q'|+|p'+q'|)(1+O(|p'|)+O(|q'|)),\\ Z=O(|p'|^2)+O(|q'|^2)+O(|p'+q'|^2),\quad \frac{m_p}{\xi_p}=O(|p'|),\quad \frac{m_q}{\xi_q}=O(|q'|),\quad \frac{m_F}{\xi_F}=O(|p'+q'|).\end{gathered} \tag{2.17}$$

In addition, the $O(\cdot)$ factors in (2.17) are analytic functions of $|p'|$, $|q'|$ and $|p'+q'|$. Note that, since $|\cdot|$ is not an analytic function (its second derivative diverges at 0), the $O(\cdot)$ factors are *not* analytic functions of p', q' or $p'+q'$. Therefore, if $W=-\omega3\sqrt{3}t_2\sin\phi$, then

$$\mathcal{I}_-(p,q):=\frac{27}{64\pi^4}\frac{(\xi_p+\xi_q+\xi_F)(\frac{m_p}{\xi_p}+\frac{m_q}{\xi_q}-\frac{m_F}{\xi_F}-\frac{m_pm_qm_F}{\xi_p\xi_q\xi_F})Z}{(Z^2-(\xi_p+\xi_q+\xi_F)^2)^2} \tag{2.18}$$

- is smooth as long as $p\neq p_F^\omega$ and $q\neq p_F^\omega$ and $p+q\neq 2p_F^\omega$,
- is bounded for all p,q,
- its derivatives diverge if $p=p_F^\omega$ or $q=p_F^\omega$ or $p+q=2p_F^\omega$.

Similarly, if $W=-\omega3\sqrt{3}t_2\sin\phi$, then

$$\mathcal{I}_+(p,q):=\frac{27}{128\pi^4}\frac{\left(1-\frac{m_pm_F}{\xi_p\xi_F}-\frac{m_qm_F}{\xi_q\xi_F}+\frac{m_pm_q}{\xi_p\xi_q}\right)(Z^2+(\xi_p+\xi_q+\xi_F)^2)}{(Z^2-(\xi_p+\xi_q+\xi_F)^2)^2} \tag{2.19}$$

- is smooth as long as $p\neq p_F^\omega$ and $q\neq p_F^\omega$ and $p+q\neq 2p_F^\omega$,
- diverges if $p=p_F^\omega$ and $q=p_F^\omega$ (it would remain bounded if it were multiplied by $|p-p_F^\omega|\cdot|q-p_F^\omega|$),
- is bounded for all $(p,q)\neq(p_F^\omega,p_F^\omega)$,
- its derivatives diverge if $p=p_F^\omega$ or $q=p_F^\omega$ or $p+q=2p_F^\omega$.

In the next section, we will regularize these singularities by changing performing an appropriate change of variables.

2.1.4. Sunrise coordinates

In this section, we will show how to regularize the singularities mentioned in the previous section. We assume throughout this section that $W=-\omega3\sqrt{3}t_2\sin\phi$ (if this is not the case, then there are no singularities).

Warning: As it is set up here, **this computation is only accurate if ϕ is not too close to 0** (see the remark on p. 9).

While $\mathcal{I}_-$ and $|p-p_F^\omega||q-p_F^\omega|\mathcal{I}_+$ are singular functions of p and q (because of the divergence of the second derivative of $|p-p_F^\omega|$), they can be re-expressed as smooth functions of p, q,

$\rho := |p - p_F^\omega|$, $r := |q - p_F^\omega|$ and $\gamma := |p + q - 2p_F^\omega|$. We will, therefore, change to the *sunrise* coordinates, described in appendix A2, which, by lemma A2.1, regularize the singularities of $\mathcal{I}_-$ and $\mathcal{I}_+$. However, the sunrise coordinates are only defined for rotationally symmetric integration regions, so we will have to split the integration regions, and note that in the regions where we cannot change to sunrise coordinates, it suffices to use polar coordinates.

Let

$$\mathcal{B}_\pm := \mathcal{B} \cap \{(k_1, k_2) \in \mathcal{B} \mid \pm k_2 > 0\} \tag{2.20}$$

and

$$\mathcal{B}_\pm^{(F)} := \{p_F^\pm + k',\ |k'| < R\}, \quad R := \frac{2\pi}{3\sqrt{3}}, \quad \mathcal{B}_\pm^{(R)} := \mathcal{B}_\pm \setminus \mathcal{B}_\pm^{(F)} \tag{2.21}$$

($\mathcal{B}_\pm^{(F)}$ is the largest disk that is included in $\mathcal{B}_\pm$). As is discussed below (see the remark on p. 11), it is inconvenient to sharply split the integral, so we will use a smooth cut-off function instead: we define, for $\tau \in (0,1)$, $\chi_\tau : [0, \infty) \to [0,1]$:

$$\chi_\tau(x) := \begin{cases} \frac{e^{-\frac{1-\tau}{1-x}}}{e^{-\frac{1-\tau}{x-\tau}} + e^{-\frac{1-\tau}{1-x}}(1 - e^{-\frac{1-\tau}{x-\tau}})} & \text{if } x \in (\tau, 1) \\ 0 & \text{if } x \in [0, \tau] \cup [1, \infty) \end{cases} \tag{2.22}$$

which is equal to 1 if $x \leqslant \tau$, and to 0 if $x \geqslant 1$, and is $\mathcal{C}^\infty$. In addition, one can prove that χ_τ is a class-2 Gevrey function, that is, $\exists C_0, C > 0$ such that for all $x \in [0, \infty)$ and $n \in \mathbb{N}$,

$$\sup \left| \frac{d^n \chi_\tau}{dx^n} \right| \leqslant C_0 C^n (n!)^2. \tag{2.23}$$

Note that C_0 and C depend on τ, and diverge as $\tau \to 1$. We will fix $\tau = \frac{1}{2}$ in the following.

Remark: By introducing such a cutoff function, the integrands will no longer be a analytic, but class-2 Gevrey functions. By lemma A3.1 (see appendix A3), the error of the numerical integration scheme nevertheless decays as an exponential in $\sqrt{N}$ where N denotes the order of the quadrature.

Let, for $p \in \mathcal{B}$

$$f_\omega^{(F)}(p) := \chi_{\frac{1}{2}}\left(\frac{|p - p_F^\omega|_{\mathcal{B}}}{R} \right) \qquad f_\omega^{(R)}(p) := 1 - f_\omega^{(F)}(p) \tag{2.24}$$

where the choice $\tau = \frac{1}{2}$ is arbitrary (any other value would do, as long as it is not too close to 0 or 1), we recall that $R := \frac{2\pi}{3\sqrt{3}}$, and $|\cdot|_{\mathcal{B}}$ denotes the periodic Euclidian norm on $\mathcal{B}$:

$$|k|_{\mathcal{B}} := \min\{|k + n_1 G_+ + n_2 G_-|,\ (n_1, n_2) \in \mathbb{Z}^2\}, \quad G_\pm := (\tfrac{2\pi}{3}, \pm\tfrac{2\pi}{\sqrt{3}}). \tag{2.25}$$

We then split

$$z_1 \mp z_2 = A_{F,F}^{(\mp)} + 2A_{R,F}^{(\mp)} + A_{R,R}^{(\mp)} \tag{2.26}$$

where

$$\begin{aligned} A_{F,F}^{(\mp)} &:= \int_{\mathcal{B}_\omega^{(F)}} dp \int_{\mathcal{B}_\omega^{(F)}} dq\ f_\omega^{(F)}(p) f_\omega^{(F)}(q)\ \mathcal{I}_\mp(p,q) \\ A_{R,F}^{(\mp)} &:= \int_{\mathcal{B}} dp \int_{\mathcal{B}_\omega^{(F)}} dq\ f_\omega^{(R)}(p) f_\omega^{(F)}(q)\ \mathcal{I}_\mp(p,q) \\ A_{R,R}^{(\mp)} &:= \int_{\mathcal{B}} dp \int_{\mathcal{B}} dq\ f_\omega^{(R)}(p) f_\omega^{(R)}(q)\ \mathcal{I}_\mp(p,q) \end{aligned} \tag{2.27}$$

in which we used the symmetry $\mathcal{I}_\mp(p,q) = \mathcal{I}_\mp(q,p)$. We will change to sunrise coordinates in $A_{F,F}$ and to polar coordinates in $A_{R,F}$ and $A_{R,R}$.

1 - The integrand of $A_{F,F}^{(\mp)}$ has the same singularities as $\mathcal{I}_\mp$, which we regularize by changing to *sunrise coordinates*. Since $\mathcal{B}_\omega^{(F)}$ is a disk, these coordinates are well defined (see lemma A2.1). In order to get rid of factors of π, we first rescale p and q by $R = \frac{2\pi}{3\sqrt{3}}$, and find

$$A_{F,F}^{(\mp)} = 2\int_0^1 d\rho \int_0^{2\pi} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\psi \int_0^1 dz\ \Sigma f_{\omega,1}^{(F)}(\sigma)\Sigma f_{\omega,2}^{(F)}(\sigma)\Sigma J(\sigma)\Sigma\mathcal{I}_\mp(\sigma) \tag{2.28}$$

with $\sigma \equiv (\rho,\theta,\psi,z)$,

$$\Sigma J(\sigma) = 4\rho^3 \frac{\bar{r}(1+\bar{r}\cos(2\psi))}{(1+\cos\psi)\sqrt{1+\bar{r}\cos^2\psi}}, \tag{2.29}$$

where $\bar{r}$ is defined in (A2.12),

$$\Sigma f_{\omega,1}^{(F)}(\sigma) := \chi_{\frac{1}{2}}(\rho), \quad \Sigma f_{\omega,2}^{(F)}(\sigma) := \chi_{\frac{1}{2}}(\rho\bar{r}), \tag{2.30}$$

$$\begin{aligned}\Sigma\mathcal{I}_-(\sigma) &:= \frac{1}{108}\frac{(\Sigma\xi_p+\Sigma\xi_q+\Sigma\xi_F)(\frac{\Sigma m_p}{\Sigma\xi_p}+\frac{\Sigma m_q}{\Sigma\xi_q}-\frac{\Sigma m_F}{\Sigma\xi_F}-\frac{\Sigma m_p\Sigma m_q\Sigma m_F}{\Sigma\xi_p\Sigma\xi_q\Sigma\xi_F})\Sigma Z}{(\Sigma Z^2-(\Sigma\xi_p+\Sigma\xi_q+\Sigma\xi_F)^2)^2}\\ \Sigma\mathcal{I}_+(\sigma) &:= \frac{1}{216}\frac{\left(1-\frac{\Sigma m_p\Sigma m_F}{\Sigma\xi_p\Sigma\xi_F}-\frac{\Sigma m_q\Sigma m_F}{\Sigma\xi_q\Sigma\xi_F}+\frac{\Sigma m_p\Sigma m_q}{\Sigma\xi_p\Sigma\xi_q}\right)(\Sigma Z^2+(\Sigma\xi_p+\Sigma\xi_q+\Sigma\xi_F)^2)}{(\Sigma Z^2-(\Sigma\xi_p+\Sigma\xi_q+\Sigma\xi_F)^2)^2}\end{aligned} \tag{2.31}$$

in which

$$\begin{aligned}\Sigma\xi_p &:= \bar{\xi}\left(\sqrt{3}+\rho\cos\theta,\omega+\omega\rho\sin\theta\right), \quad \Sigma\xi_q := \bar{\xi}\left(\sqrt{3}+\rho\bar{r}\cos(\theta+\varphi),\omega+\omega\rho\bar{r}\sin(\theta+\varphi)\right),\\ \Sigma\xi_F &:= \bar{\xi}\left(\sqrt{3}+\rho(\cos\theta+\bar{r}\cos(\theta+\varphi)),\omega+\omega\rho(\sin(\theta)+\bar{r}\sin(\theta+\varphi))\right),\end{aligned} \tag{2.32}$$

where φ is defined in (A2.13), and

$$\begin{aligned}\bar{\xi}(\bar{k}) &:= \sqrt{\bar{m}^2(\bar{k})+2t_1^2\bar{\alpha}_1(\bar{k})}, \quad \bar{\zeta}(\bar{k}) := 2t_2\cos\phi\bar{\alpha}_1(\bar{k}), \quad \bar{m}(\bar{k}) := W-2t_2\sin\phi\bar{\alpha}_2(\bar{k}),\\ \bar{\alpha}_1(\bar{k}_1,\bar{k}_2) &:= 2\cos\left(\frac{\pi}{3}\bar{k}_2\right)\left(\cos\left(\frac{\pi}{\sqrt{3}}\bar{k}_1\right)+\cos\left(\frac{\pi}{3}\bar{k}_2\right)\right)+\frac{1}{2},\\ \bar{\alpha}_2(\bar{k}_1,\bar{k}_2) &:= 2\sin\left(\frac{\pi}{3}\bar{k}_2\right)\left(\cos\left(\frac{\pi}{\sqrt{3}}\bar{k}_1\right)-\cos\left(\frac{\pi}{3}\bar{k}_2\right)\right),\end{aligned} \tag{2.33}$$

$$\begin{aligned}\Sigma m_p &:= \bar{m}\left(\sqrt{3}+\rho\cos\theta,\omega+\omega\rho\sin\theta\right), \quad \Sigma m_q := \bar{m}\left(\sqrt{3}+\rho\bar{r}\cos(\theta+\varphi),\omega+\omega\rho\bar{r}\sin(\theta+\varphi)\right),\\ \Sigma m_F &:= \bar{m}\left(\sqrt{3}+\rho(\cos\theta+\bar{r}\cos(\theta+\varphi)),\omega+\omega\rho(\sin(\theta)+\bar{r}\sin(\theta+\varphi))\right),\end{aligned} \tag{2.34}$$

and

$$\Sigma Z := \Sigma\zeta_p+\Sigma\zeta_q-\Sigma\zeta_F \tag{2.35}$$

with

$$\begin{aligned}\Sigma\zeta_p &:= \bar{\zeta}\left(\sqrt{3}+\rho\cos\theta,\omega+\omega\rho\sin\theta\right), \quad \Sigma\zeta_q := \bar{\zeta}\left(\sqrt{3}+\rho\bar{r}\cos(\theta+\varphi),\omega+\omega\rho\bar{r}\sin(\theta+\varphi)\right),\\ \Sigma\zeta_F &:= \bar{\zeta}\left(\sqrt{3}+\rho(\cos\theta+\bar{r}\cos(\theta+\varphi)),\omega+\omega\rho(\sin(\theta)+\bar{r}\sin(\theta+\varphi))\right).\end{aligned} \tag{2.36}$$

Let us now check that the functions $\Sigma J\Sigma\mathcal{I}_\mp$ and $\Sigma f_{\omega,i}$ are smooth. This is almost a direct consequence of lemma A2.1 and (2.17), if not for the fact that the sunrise coordinates ignore the periodic nature of the Brillouin zone $\mathcal{B}$. If $p+q-p_F^\omega$ were equal to $p_F^\omega+(n_1G_+ + n_2G_-)$ with $G_\pm = (\frac{2}{\pi}3, \pm\frac{2\pi}{\sqrt{3}})$ and $(n_1,n_2)\in\mathbb{Z}^2\setminus\{(0,0)\}$ then $\mathcal{I}_\mp(p,q)$ would have a singularity that is not regularized by the sunrise coordinates. However, one readily checks that this cannot happen when

p and q are in $\mathcal{B}_\omega^{(F)}$. All in all, $\Sigma J \Sigma \mathcal{I}_\mp$ is an analytic function on the closure of the integration domain, and $\Sigma f_{\omega,i}^{(F)}$ is a class-2 Gevrey function.

Remark: In the discussion above, we assumed that $\mathcal{I}(p,q)$ is not singular at $p_F^{-\omega}$, which is only true if $\phi \neq 0$. If ϕ is small, then the derivatives of $\mathcal{I}(p,q)$ may be very large if one of p, q or $p+q-p_F^\omega$ is close to $p_F^{-\omega}$. When p and q are in $\mathcal{B}_\omega^{(F)}$, $p+q-p_F^\omega$ may be arbitrarily close to $p_F^{-\omega}$, which means that ϕ must be sufficiently far from 0 for the accuracy of the computation described above to be good.

Finally, using the $\frac{2\pi}{3}$ rotation symmetry, we rewrite

$$A_{F,F}^{(\mp)} = 6\int_0^1 d\rho \int_{-\frac{\pi}{6}}^{\frac{\pi}{2}} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\psi \int_0^1 dz\ \Sigma f_{\omega,1}^{(F)}(\sigma)\Sigma f_{\omega,2}^{(F)}(\sigma)\Sigma J(\sigma)\Sigma\mathcal{I}_\mp(\sigma). \tag{2.37}$$

2 - The integrand of $A_{R,F}^{(\mp)}$ is only singular if $q = p_F^\omega$ or $p+q-p_F^\omega = p_F^\omega$, because $|p-p_F^\omega|_{\mathcal{B}} > \frac{R}{2}$. We regularize these singularities by switching to polar coordinates corresponding to q and $p+q-p_F^\omega$, which we denote by (r,θ,ρ,φ): if $p+q-p_F^\omega \in \mathcal{B}_\nu$,

$$q = p_F^\omega + \omega\frac{2\pi}{3\sqrt{3}}\rho(\cos\theta,\sin\theta), \quad p+q-p_F^\omega = p_F^\nu + \nu\frac{2\pi}{3\sqrt{3}}r(\cos\varphi,\sin\varphi) \tag{2.38}$$

in terms of which

$$A_{R,F}^{(\mp)} = \sum_{\nu=\pm}\int_0^{2\pi} d\theta \int_0^{2\pi} d\varphi \int_0^1 dr \int_0^{R(\varphi)} d\rho\ \rho r \Pi f_\omega^{(R)}(\varpi)\Pi f_\omega^{(F)}(\varpi)\Pi\mathcal{I}_\mp(\varpi) \tag{2.39}$$

with $\varpi \equiv (r,\theta,\rho,\varphi)$,

$$\Pi f_\omega^{(R)}(\varpi) := \chi_{\frac{1}{2}}\left(|(\rho\cos\varphi - r\cos\theta,\ \nu-\omega+\nu\rho\sin\varphi-\omega r\sin\theta)|_{\mathbb{T}}\right), \quad \Pi f_\omega^{(F)}(\varpi) := \chi_{\frac{1}{2}}(r) \tag{2.40}$$

where

$$|\bar{k}|_{\mathbb{T}} := \min\left\{|\bar{k} + n_1(\sqrt{3},1) + n_2(\sqrt{3},-1)|,\ (n_1,n_2)\in\mathbb{Z}^2\right\}, \tag{2.41}$$

$$\begin{gathered}\Pi\mathcal{I}_-(\varpi) := \frac{1}{108}\frac{(\Pi\xi_p+\Pi\xi_q+\Pi\xi_F)(\frac{\Pi m_p}{\Pi\xi_p}+\frac{\Pi m_q}{\Pi\xi_q}-\frac{\Pi m_F}{\Pi\xi_F}-\frac{\Pi m_p\Pi m_q\Pi m_F}{\Pi\xi_p\Pi\xi_q\Pi\xi_F})\Pi Z}{(\Pi Z^2-(\Pi\xi_p+\Pi\xi_q+\Pi\xi_F)^2)^2}\\ \Pi\mathcal{I}_+(\varpi) := \frac{1}{216}\frac{\left(1-\frac{\Pi m_p\Pi m_F}{\Pi\xi_p\Pi\xi_F}-\frac{\Pi m_q\Pi m_F}{\Pi\xi_q\Pi\xi_F}+\frac{\Pi m_p\Pi m_q}{\Pi\xi_p\Pi\xi_q}\right)(\Pi Z^2+(\Pi\xi_p+\Pi\xi_q+\Pi\xi_F)^2)}{(\Pi Z^2-(\Pi\xi_p+\Pi\xi_q+\Pi\xi_F)^2)^2}\end{gathered} \tag{2.42}$$

in which

$$\begin{gathered}\Pi\xi_q := \bar{\xi}\left(\sqrt{3}+r\cos\theta,\omega+\omega r\sin\theta\right), \quad \Pi\xi_F := \bar{\xi}\left(\sqrt{3}+\rho\cos\varphi,\nu+\nu\rho\sin\varphi\right),\\ \Pi\xi_p := \bar{\xi}\left(\sqrt{3}-r\cos\theta+\rho\cos\varphi),\nu-\omega r\sin\theta+\nu\rho\sin\varphi\right),\end{gathered} \tag{2.43}$$

where $\bar{\xi}$ is defined in (2.33),

$$\begin{gathered}\Pi m_q := \bar{m}\left(\sqrt{3}+r\cos\theta,\omega+\omega r\sin\theta\right), \quad \Pi m_F := \bar{m}\left(\sqrt{3}+\rho\cos\varphi,\nu+\nu\rho\sin\varphi\right),\\ \Pi m_p := \bar{m}\left(\sqrt{3}-r\cos\theta+\rho\cos\varphi),\nu-\omega r\sin\theta+\nu\rho\sin\varphi\right),\end{gathered} \tag{2.44}$$

where $\bar{m}$ is defined in (2.33),

$$\Pi Z := \Pi\zeta_p + \Pi\zeta_q - \Pi\zeta_F \tag{2.45}$$

with

$$\Pi\zeta_q := \bar\zeta\left(\sqrt{3}+r\cos\theta,\omega+\omega r\sin\theta\right), \quad \Pi\zeta_F := \bar\zeta\left(\sqrt{3}+\rho\cos\varphi,\nu+\nu\rho\sin\varphi\right),$$
$$\Pi\zeta_p := \bar\zeta\left(\sqrt{3}-r\cos\theta+\rho\cos\varphi),\nu-\omega r\sin\theta+\nu\rho\sin\varphi\right) \tag{2.46}$$

where $\bar\zeta$ is defined in (2.33), and

$$R(\theta) = \begin{cases} \frac{1}{\cos(\theta-\frac{\pi}{6})} & \text{if } \theta\in\left[-\frac{\pi}{6},\frac{\pi}{2}\right] \\ \frac{1}{\cos(\theta-\frac{5\pi}{6})} & \text{if } \theta\in\left[\frac{\pi}{2},\frac{7\pi}{6}\right] \\ \frac{1}{\cos(\theta+\frac{\pi}{2})} & \text{if } \theta\in\left[\frac{7\pi}{6},\frac{11\pi}{6}\right]. \end{cases} \tag{2.47}$$

Note that $R(\theta)$ is smooth by parts, so, in order to keep the accuracy of the computation high, we must split the integral over φ:

$$A^{(\mp)}_{R,F} = 3\sum_{\nu=\pm}\int_0^{2\pi}d\theta\int_{-\frac{\pi}{6}}^{\frac{\pi}{2}}d\varphi\int_0^1 dr\int_0^{R(\varphi)}d\rho\ \rho r\Pi f^{(R)}_\omega(\varpi)\Pi f^{(F)}_\omega(\varpi)\Pi\mathcal{I}_\mp(\varpi) \tag{2.48}$$

In which we used the symmetry under $\frac{2\pi}{3}$ rotations of p and q.

By (2.17) and the fact that $|p-p_F^\omega|_{\mathcal{B}} > \frac{R}{2}$ on the support of $f^{(R)}_\omega$, $\rho r\Pi\mathcal{I}_\mp$ is an analytic function on the closure of the integration domain, and $\Pi f^{(F)}_\omega$ and $\Pi f^{(R)}_\omega$ are class-2 Gevrey functions.

Remark: In order to regularize the singularity at $p+q-p_F^\omega = p_F^\omega$, we had to change variables to $(q, p+q-p_F^\omega)$. If, instead of the smooth cutoff function f_ω, we had used a step function, the integration region for $p+q-p_F^\omega$ would have been $\mathcal{B}$ minus a disk centered around q of radius R. This creates trouble, since the parametrization of this disk is singular when p_F^ω tends to the boundary of the disk. The reason for which we have used a smooth cutoff function is to avoid this problem.

3 - The integrand of $A^{(\mp)}_{R,R}$ is only singular if $p+q-p_F^\omega = p_F^\omega$, because $|p-p_F^\omega|_{\mathcal{B}} > \frac{R}{2}$ and $|q-p_F^\omega|_{\mathcal{B}} > \frac{R}{2}$. We regularize this singularity by switching to polar coordinates corresponding to q and $p+q-p_F^\omega$, which we denote by (r,θ,ρ,φ): if $q\in\mathcal{B}_\eta$ and $p+q-p_F^\omega\in\mathcal{B}_\nu$, then we define

$$q = p_F^\eta + \eta\frac{2\pi}{3\sqrt{3}}r(\cos\theta,\sin\theta), \quad p+q-p_F^\omega = p_F^\nu + \nu\frac{2\pi}{3\sqrt{3}}\rho(\cos\varphi,\sin\varphi) \tag{2.49}$$

in terms of which

$$A^{(\mp)}_{R,R} = \sum_{\eta,\nu=\pm}\int_0^{2\pi}d\theta\int_0^{2\pi}d\varphi\int_0^{R(\theta)}dr\int_0^{R(\varphi)}d\rho\ \rho r\Xi f^{(R)}_{\omega,1}(\varpi)\Xi f^{(R)}_{\omega,2}(\varpi)\Xi\mathcal{I}_\mp(\varpi) \tag{2.50}$$

with $\varpi\equiv(r,\theta,\rho,\varphi)$,

$$\Xi f^{(R)}_{\omega,1}(\varpi) := \chi_{\frac12}\left(|(\rho\cos\varphi-r\cos\theta,\ \nu-\eta+\nu\rho\sin\varphi-\eta r\sin\theta)|_{\mathbb{T}}\right),$$
$$\Xi f^{(R)}_{\omega,2}(\varpi) := \chi_{\frac12}\left(|(r\cos\theta,\ \eta-\omega+\eta r\sin\theta)|_{\mathbb{T}}\right) \tag{2.51}$$

where

$$|\bar k|_{\mathbb{T}} := \min\left\{|\bar k + n_1(\sqrt{3},1)+n_2(\sqrt{3},-1)|,\ (n_1,n_2)\in\mathbb{Z}^2\right\}, \tag{2.52}$$

$$\Xi\mathcal{I}_-(\varpi) := \frac{1}{108}\frac{(\Xi\xi_p+\Xi\xi_q+\Xi\xi_F)(\frac{\Xi m_p}{\Xi\xi_p}+\frac{\Xi m_q}{\Xi\xi_q}-\frac{\Xi m_F}{\Xi\xi_F}-\frac{\Xi m_p\Xi m_q\Xi m_F}{\Xi\xi_p\Xi\xi_q\Xi\xi_F})\Xi Z}{(\Xi Z^2-(\Xi\xi_p+\Xi\xi_q+\Xi\xi_F)^2)^2}$$
$$\Xi\mathcal{I}_+(\varpi) := \frac{1}{216}\frac{\left(1-\frac{\Xi m_p\Xi m_F}{\Xi\xi_p\Xi\xi_F}-\frac{\Xi m_q\Xi m_F}{\Xi\xi_q\Xi\xi_F}+\frac{\Xi m_p\Xi m_q}{\Xi\xi_p\Xi\xi_q}\right)(\Xi Z^2+(\Xi\xi_p+\Xi\xi_q+\Xi\xi_F)^2)}{(\Xi Z^2-(\Xi\xi_p+\Xi\xi_q+\Xi\xi_F)^2)^2} \tag{2.53}$$

in which

$$\Xi\xi_q := \bar\xi\left(\sqrt3+r\cos\theta,\eta+\eta r\sin\theta\right),\quad \Xi\xi_F := \bar\xi\left(\sqrt3+\rho\cos\varphi,\nu+\nu\rho\sin\varphi\right),$$
$$\Xi\xi_p := \bar\xi\left(\sqrt3-r\cos\theta+\rho\cos\varphi),\nu+\omega-\eta-\eta r\sin\theta+\nu\rho\sin\varphi\right), \tag{2.54}$$

where $\bar\xi$ is defined in (2.33),

$$\Xi m_q := \bar m\left(\sqrt3+r\cos\theta,\eta+\eta r\sin\theta\right),\quad \Xi m_F := \bar m\left(\sqrt3+\rho\cos\varphi,\nu+\nu\rho\sin\varphi\right),$$
$$\Xi m_p := \bar m\left(\sqrt3-r\cos\theta+\rho\cos\varphi),\nu+\omega-\eta-\eta r\sin\theta+\nu\rho\sin\varphi\right), \tag{2.55}$$

where $\bar m$ is defined in (2.33),

$$\Xi Z := \Xi\zeta_p+\Xi\zeta_q-\Xi\zeta_F \tag{2.56}$$

with

$$\Xi\zeta_q := \bar\zeta\left(\sqrt3+r\cos\theta,\eta+\eta r\sin\theta\right),\quad \Xi\zeta_F := \bar\zeta\left(\sqrt3+\rho\cos\varphi,\nu+\nu\rho\sin\varphi\right),$$
$$\Xi\zeta_p := \bar\zeta\left(\sqrt3-r\cos\theta+\rho\cos\varphi),\nu+\omega-\eta-\eta r\sin\theta+\nu\rho\sin\varphi\right) \tag{2.57}$$

where $\bar\zeta$ is defined in (2.33), and R is defined in (2.47). Here, again, since $R(\theta)$ is only smooth by parts, we must split the integral over θ and φ:

$$A^{(\mp)}_{R,R} = 3\sum_{\eta,\nu=\pm}\sum_{a=0,1,2}\int_{(4a-1)\frac{\pi}{6}}^{(4a+3)\frac{\pi}{6}}d\theta\int_{-\frac{\pi}{6}}^{\frac{\pi}{2}}d\varphi\int_0^{R(\theta)}dr\int_0^{R(\varphi)}d\rho\ \rho r\Xi f^{(R)}_{\omega,1}(\varpi)\Xi f^{(R)}_{\omega,2}(\varpi)\Xi\mathcal{I}_\mp(\varpi) \tag{2.58}$$

In which we used the symmetry under $\frac{2\pi}{3}$ rotations of p and q.

By (2.17) and the fact that $|p-p_F^\omega|_{\mathcal{B}}>\frac{R}{2}$ and $|q-p_F^\omega|_{\mathcal{B}}>\frac{R}{2}$ on the support of $f_\omega^{(R)}$, $r\Xi\mathcal{I}_\mp$ is an analytic function on the closure of the integration domain, and $\Xi f^{(R)}_{\omega,1}$ and $\Xi f^{(R)}_{\omega,2}$ are class-2 Gevrey functions.

2.2. Strategy of the numerical computation

The integrations are carried out using Gauss-Legendre quadratures (see section 3.2).

2.3. Usage and examples

We will now describe some basic usage cases of `hhtop z1-z2`. For a full description of the options of `hhtop`, see the `man` page.

2.3.1. Basic usage

The value of the parameters can be set via the `-p` flag. Here is an example

```
hhtop z1-z2 -p "omega=1;t1=1.;t2=.1;phi=1;"
hhtop z1+z2 -p "omega=1;t1=1.;t2=.1;phi=1;"
```

The parameters that are not specified by the `-p` flag are set to their default value: $\omega=1$, $t_1=1$, $t_2=0.1$, $\phi=\frac{\pi}{2}$, $W=\omega3\sqrt{3}t_2\sin\phi$.

2.3.2. Precision of the computation

The precision of the computation can be controlled by three parameters: the precision of the numbers manipulated by `hhtop` (set via the `-P` flag, see section 3.3), the order of the integration, and the tolerance of the computation of abcissa and weights.

1 - Order of the integration. The order of the integration, that is, the value of the number N introduced in section 3.2, can be specified via the `-O` flag. Its default value is 10. The difference of the value of the integral at different orders is a good measure of the numerical error. Example:

```
hhtop z1-z2 -O 30
hhtop z1+z2 -O 30
```

2 - Tolerance of the abcissa and weights. A Newton scheme is used to compute the abcissa and weights of the Gauss-Legendre integration. The scheme halts when the difference $|x_{n+1} - x_n|$ (see section 3.1) is smaller than a number, called the *tolerance* of the algorithm, or when the toal number of steps exceeds a given threshold. The tolerance can be set via the `-t` flag, and the maximal number of steps via the `-N` flag. Their default values are 10^{-11} and 1000000. If the tolerance or the maximal number of steps are too small, and the precision of multi-precision floats is too low, then the iteration may not converge. Example:

```
hhtop z1-z2 -t 1e-30 -N 2000000 -O 100 -P 256
hhtop z1+z2 -t 1e-30 -N 2000000 -O 100 -P 256
```

2.3.3. Using double precision floats instead of multi-precision floats

Using the `-D` command-line flag, `hhtop` can be instructed to use `long double`'s instead of MPFR floats. Whereas one then loses the ability of adjusting the precision, the computation time can be drastically reduced. Example:

```
hhtop -D z1-z2 -p "sinphi=1.;"
hhtop -D z1+z2 -p "sinphi=1.;"
```

The precision of `long doubles` is compiler dependent, see section 3.3.

3. Algorithms

In this section, we describe the algorithms used by `hhtop`. Their implementation is provided by the `libinum` library.

3.1. Newton scheme

The Newton algorithm is used to compute roots: given a real function f and an initial guess x_0 for the root, the Newton scheme produces a sequence (x_n):

$$x_{n+1} := x_n - \frac{f(x_n)}{\partial_x f(x_n)} \tag{3.1}$$

which, provided the sequence converges, it tends to a solution of $f(x) = 0$, with a quadratic rate of convergence

$$|x_{n+1} - x_n| \leqslant c_n |x_n - x_{n-1}|^2 \tag{3.2}$$

where

$$c_n := \frac{1}{2} \frac{\sup_{x\in[x_{n+1},x_n]} |\partial_x^2 f(x)|}{\inf_{x\in[x_{n+1},x_n]} |\partial_x f(x)|}. \tag{3.3}$$

3.2. Gauss-Legendre integration

The Gauss-Legendre method allows us to compute

$$\int_{-1}^{1} dx\ f(x) \tag{3.4}$$

for $f : [-1, 1] \to \mathbb{R}$. Having fixed an *order* $N \in \mathbb{N} \setminus \{0\}$, let $\{x_1, \cdots, x_N\}$ denote the set of roots of the N-th Legendre polynomial P_N,and let

$$w_i = \frac{2}{(1 - x_i^2) P_N'(x_i)} \tag{3.5}$$

for $i \in \{1, \cdots, N\}$. One can show that, if f is a polynomial of order $\leqslant 2N - 1$, then

$$\int_{-1}^{1} dx\ f(x) = \sum_{i=1}^{N} w_i f(x_i). \tag{3.6}$$

If f is an analytic function, then one can show that the error decays exponentially as $N \to \infty$. However, in the computation of $z_1 - z_2$ (see section 2), we use Gauss-Legendre quadratures to integrate a class-2 Gevrey function, so we will need to generalize this result. Let us first define class-s Gevrey functions on $[-1, 1]$, as $\mathcal{C}^\infty$ functions, for which there exist $C_0, C > 0$, such that $\forall n \in \mathbb{N}$,

$$\sup_{x\in[-1,1]} \left| \frac{d^n f(x)}{dx^n} \right| \leqslant C_0 C^n (n!)^s. \tag{3.7}$$

Note that the set of analytic functions on $[-1, 1]$ is equal to the set of class-1 Gevrey functions on $[-1, 1]$. We assume that $s \in \mathbb{N} \setminus \{0\}$.

The basic strategy to estimate the error

$$E_N(f) := \left| \int_{-1}^{1} dx\ f(x) - \sum_{i=1}^{N} w_i f(x) \right| \tag{3.8}$$

is to approximate f using Chebyshev polynomials, bound the error of this approximation for Gevrey functions, and use an estimate of the error when f is a Chebyshev polynomial. This is done in detail in appendix A3, and we find (see lemma A3.1)

$$E_N(f) \leqslant c_0 c_1^{s-1}(2N)^{1-\frac{1}{s}} e^{-b(2N)^{\frac{1}{s}}} s!. \tag{3.9}$$

3.3. Precision

The numerical values manipulated by `hhtop` are represented as multi-precision floats (using the GNU MPFR library). The number of bits allocated to each number, that is, the number of digits used in the computation, can be specified using the `-P` flag. The default precision is 53 bits. Example:

```
hhtop phase -P 128
```

This behavior can be changed using the `-D` flag, in which case the numerical values are represented as `long double`, which have a fixed precision, but yield faster computation times. Example:

```
hhtop -D phase
```

The precision of `long double`'s is compiler-dependent, and can be checked using the `-Vv` flag:

```
hhtop -Vv
```

Using the GNU GCC compiler, version 5.3.0, on the `x86-64` architecture, the precision of `long double`'s is 64.

Appendices

A1. Proof of (1.11)

In this appendix, we show that (1.10) holds, then (1.11) does as well. To alleviate the notation, we will drop the ${}_{t_1,t_2,W,\phi}$ indices as well as the '(k)'. We have

$$\xi^2 - \zeta^2 = m^2 + t_1^2|\Omega|^2 - 4t_2^2\cos^2\phi\alpha_1^2 \tag{A1.1}$$

which, using $|\Omega|^2 = 2\alpha_1$, becomes

$$\xi^2 - \zeta^2 = m^2 + 2\alpha_1(t_1^2 - 2t_2^2\alpha_1). \tag{A1.2}$$

Furthermore, $0 \leqslant \alpha_1 \leqslant \frac{9}{2}$ (both 0 and $\frac{9}{2}$ are reached, respectively at 0 and $p_F := (\frac{2\pi}{3}, \frac{2\pi}{3\sqrt{3}})$). This implies that $\xi^2 > \zeta^2$.

A2. Sunrise coordinates

In this appendix, we discuss the *sunrise* coordinates, which are used to compute sunrise Feynman diagrams. Such diagrams give rise to an integral of the form

$$\int dpdq\ F(p,q,|p|,|q|,|p+q|) \tag{A2.1}$$

where $\rho r F(p,q,\rho,r,\gamma)$ is an analytic function of p, q, ρ, r and γ, and

$$|(p_1,p_2)| := \sqrt{p_1^2 + p_2^2}. \tag{A2.2}$$

However, since $|p|$, $|q|$ and $|p+q|$ are not analytic, the derivatives of $F(p,q,|p|,|q|,|p+q|)$ are, typically, unbounded, which can cause the error in the numerical evaluation of the integral uncontrollably large. In order to avoid this problem, we introduce coordinates, (ρ,θ,ψ,z), called *sunrise coordinated*, which are such that p, q, $|p|$, $|q|$, $|p+q|$, as well as the Jacobian of the change of variables, are analytic functions of (ρ,θ,ψ,z). Expressed using the sunrise coordinates, the integral of F can be computed with good numerical accuracy.

Remark: Note that if, instead of the sunrise coordinates, one used the (simpler) polar coordinates $p = \rho(\cos\theta,\sin\theta)$ and $q = r(\cos\varphi,\sin\varphi)$, then $|p+q| = \sqrt{\rho^2 + r^2 + 2\rho r\cos(\theta-\varphi)}$, which has a divergent second derivative at $(\rho,\theta) = (r,-\varphi)$. Polar coordinates, therefore, do not do the trick.

Remark: The sunrise coordinates are introduced in the following lemma, which is only stated for the case $|p| > |q|$. The integration over the regime $|q| < |p|$ can be performed by exchanging p and q.

Lemma A2.1

Let $\mathcal{B}_R := \{p \in \mathbb{R}^2,\ |p| < R\}$. We define the map $\mathcal{S}$

$$\begin{array}{rrcl} \mathcal{S}: & \{(p,q)\in\mathcal{B}_R^2,\ |p|>|q|\} & \longrightarrow & (0,R)\times[0,2\pi)\times[-\frac{\pi}{2},\frac{\pi}{2}]\times(0,1) \\ & (p,q) & \longmapsto & (\rho,\theta,\psi,z) \end{array} \tag{A2.3}$$

with

$$\rho := |p| \in (0,R), \tag{A2.4}$$

$\theta \in [0, 2\pi)$ is the unique solution of

$$p = \rho(\cos\theta, \sin\theta), \tag{A2.5}$$

if φ denotes the angle between p and q, then $\psi \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ is the unique solution of

$$\cos\psi = \sqrt{\frac{|p+q| - |p| + |q|}{2|q|}}, \quad \text{sign}(\psi) = \text{sign}(\sin\varphi), \tag{A2.6}$$

and

$$z := 1 - \frac{1 - \sqrt{1 - \frac{|q|}{\rho}\sin^2\psi}}{1 - \cos\psi} \in (0, 1). \tag{A2.7}$$

The map $\mathcal{S}$ is invertible, its inverse is analytic, and is such that, if $(p, q) = \mathcal{S}^{-1}(\rho, \theta, \psi, z)$, then $|p|$, $|q|$ and $|p + q|$ are analytic functions of (ρ, θ, ψ, z). Furthermore, the Jacobian

$$J := \left|\det\left(\frac{\partial(p_1, p_2, q_1, q_2)}{\partial(\rho, \theta, \psi, z)}\right)\right| \tag{A2.8}$$

is an analytic function of (ρ, θ, ψ, z). In addition, $\mathcal{S}^{-1}$, $|p|$, $|q|$, $|p + q|$ and J, as functions of (ρ, θ, ψ, z), can be continued analytically to $[0, R] \times [0, 2\pi) \times [-\frac{\pi}{2}, \frac{\pi}{2}] \times [0, 1]$. Explicitly,

$$p_1 = \rho\cos\theta, \quad p_2 = \rho\sin\theta, \quad q_1 = \rho\bar{r}\cos(\theta + \varphi), \quad q_2 = \rho\bar{r}\sin(\theta + \varphi), \tag{A2.9}$$

$$|p| = \rho, \quad |q| = \rho\bar{r}, \quad |p + q| = \rho(1 + \bar{r}\cos(2\psi)) \tag{A2.10}$$

and

$$J = 4\rho^3 \frac{\bar{r}(1 + \bar{r}\cos(2\psi))}{(1 + \cos\psi)\sqrt{1 + \bar{r}\cos^2\psi}} \tag{A2.11}$$

with

$$\bar{r} := (1 - z)(1 + zh(\psi)), \quad h(\psi) := \frac{1 - \cos\psi}{1 + \cos\psi}, \quad t := 1 - (1 - z)(1 - \cos\psi), \tag{A2.12}$$

and

$$\cos\varphi := \cos(2\psi) - \frac{\bar{r}}{2}\sin^2(2\psi), \quad \sin\varphi := t\sin(2\psi)\sqrt{1 + \bar{r}\cos^2\psi}. \tag{A2.13}$$

<u>Proof</u>: In order to prove the lemma, we will compose several changes of coordinates. The *sunrise* coordinates described above are obtained by combining these intermediate changes of variables.

1 - The first, consists in changing p to polar coordinates, which yields (A2.4), (A2.5) and the first two equations of (A2.9), and contributes a factor ρ to the Jacobian:

$$\int_{\mathcal{B}_R} dp \int_{\mathcal{B}_{|p|}} dq\ F = \int_0^R d\rho \int_0^{2\pi} d\theta \int_{\mathcal{B}_\rho} dq\ \rho\ F. \tag{A2.14}$$

2 - We then change variables to

$$(\rho, \theta, q_1, q_2) \longmapsto (\rho, \theta, r, \gamma) \tag{A2.15}$$

with

$$r := |q|, \quad \gamma := |p + q| = \sqrt{\rho^2 + r^2 + 2\rho(q_1\cos\theta + q_2\sin\theta)} \tag{A2.16}$$

so that

$$\int_{\mathcal{B}_R} dp \int_{\mathcal{B}_{|p|}} dq \ F = \int_0^R d\rho \int_0^{2\pi} d\theta \int_0^\rho dr \int_{\rho-r}^{\rho+r} d\gamma \ \frac{\gamma}{|\sin\varphi|} \ F \tag{A2.17}$$

where φ is the angle between p and q:

$$\cos\varphi = \frac{\gamma^2-\rho^2-r^2}{2r\rho}, \quad |\sin\varphi| = \sqrt{1-\cos^2\varphi} = \frac{1}{2r\rho}\sqrt{4r^2\rho^2-(\gamma^2-r^2-\rho^2)^2} \tag{A2.18}$$

which we rewrite as

$$|\sin\varphi| = \frac{1}{2r\rho}\sqrt{(\rho+r+\gamma)(\rho-r+\gamma)(-\rho+r+\gamma)(\rho+r-\gamma)}. \tag{A2.19}$$

3 - We then adimensionalize r and γ, that is, we change to $\bar r, \bar\gamma$ in such a way that $\bar r, \bar\gamma \in (0,1)$:

$$\bar r := \frac{r}{\rho}, \quad \bar\gamma := \frac{\gamma-\rho+r}{2r} \tag{A2.20}$$

in terms of which

$$\int_{\mathcal{B}_R} dp \int_{\mathcal{B}_{|p|}} dq \ F = \int_0^R d\rho \int_0^{2\pi} d\theta \int_0^1 d\bar r \int_0^1 d\bar\gamma \ \frac{2\rho^3\bar r(1-\bar r+2\bar r\bar\gamma)}{|\sin\varphi|} \ F \tag{A2.21}$$

and

$$|\sin\varphi| = 2\sqrt{\bar\gamma(1-\bar\gamma)(1-\bar r+\bar r\bar\gamma)(1+\bar r\bar\gamma)}. \tag{A2.22}$$

4 - At this point, the singularities have all been shifted to $|\sin\varphi|$: p, q, $|p|$, $|q|$ and $|p+q|$ are analytic functions of ρ, $\bar r$, $\bar\gamma$, $\cos\theta$, $\sin\theta$, $\cos\varphi$ and $\sin\varphi$, and the only one of these that is singular is $\sin\varphi$, because of the square root in (A2.22). We first note that $\sqrt{1+\bar r\bar\gamma} > 1$, so that factor is not singular. In order to regularize the divergence in the other terms, we change variables to

$$\cos\psi := \sqrt{\bar\gamma}, \quad \sin\psi := \mathrm{sign}(\sin\varphi)\sqrt{1-\bar\gamma}, \quad t := \sqrt{1-\bar r(1-\bar\gamma)} \tag{A2.23}$$

after which

$$\int_{\mathcal{B}_R} dp \int_{\mathcal{B}_{|p|}} dq \ F = \int_0^R d\rho \int_0^{2\pi} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\psi \int_{\cos\psi}^1 dt \ 4\rho^3 \frac{(1-t^2)}{\sin^4\psi} \frac{\left(1+\frac{(1-t^2)}{\sin^2\psi}(2\cos^2\psi-1)\right)}{\sqrt{1+\frac{(1-t^2)}{\sin^2\psi}\cos^2\psi}} \ F. \tag{A2.24}$$

5 - Finally, we adimensionalize t:

$$z := 1 - \frac{1-t}{1-\cos\psi} \tag{A2.25}$$

so that

$$\int_{\mathcal{B}_R} dp \int_{\mathcal{B}_{|p|}} dq \ F = \int_0^R d\rho \int_0^{2\pi} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\psi \int_0^1 dz \\ 4\rho^3 \frac{(1-z)(1+zh(\psi))}{1+\cos\psi} \frac{(1+(1-z)(1+zh(\psi))(2\cos^2\psi-1))}{\sqrt{1+(1-z)(1+zh(\psi))\cos^2\psi}} \ F. \tag{A2.26}$$

6 - Equations (A2.9) through (A2.13) follow from (A2.26). The analyticity of p, q, $|p|$, $|q|$, $|p+q|$ and J is a simple comsequence of (A2.9), (A2.10) and (A2.11). $\square$

A3. Estimate of the error of Gauss-Legendre quadratures for Gevrey functions

In this appendix, we compute the error of Gauss-Legendre quadratures when used to integrate class-s Gevrey functions. A class-s Gevrey function on $[-1,1]$ is a $\mathcal{C}^\infty$ function that satisfies, $\forall n\in\mathbb{N}$,

$$\sup_{x\in[-1,1]}\left|\frac{d^nf(x)}{dx^n}\right|\leqslant C_0C^n(n!)^s. \tag{A3.1}$$

Lemma A3.1

Let f be a class-s Gevrey function with $s\in\mathbb{N}\setminus\{0\}$. There exist $c_0,c_1,b>0$, which are independent of s, and $N_0>0$, which is independent of s and f, such that, if $N\geqslant N_0$, then

$$E_N(f)\leqslant c_0c_1^{s-1}(2N)^{1-\frac1s}e^{-b(2N)^{\frac1s}}s!. \tag{A3.2}$$

In particular, if f is analytic (i.e. $s=1$), then

$$E_N(f)\leqslant c_0e^{-2bN}. \tag{A3.3}$$

Proof:

1 - We approximate f by Chebyshev polynomials:

$$f(x)=\frac{c_0}{2}+\sum_{j=1}^\infty c_jT_j(x) \tag{A3.4}$$

where T_j is the j-th Chebyshev polynomial:

$$T_j(x):=\cos(j\arccos(x)),\quad c_j:=\frac{2}{\pi}\int_0^\pi d\theta\ f(\cos\theta)\cos(j\theta). \tag{A3.5}$$

Note that (A3.4) is nothing other than the Fourier cosine series expansion of $F(\theta):=f(\cos(\theta))$, which is an even, periodic, class-s Gevrey function on $[-\pi,\pi]$, whose j-th Fourier coefficient for $j\in\mathbb{Z}$ is equal to $\frac12c_{|j|}$. Furthermore, using a well-known estimate of the decay of Fourier coefficients of class-s Gevrey functions (see e.g. [Ta87, Theorem 3.3]), there exists $b_0,b>0$ such that

$$c_j\leqslant b_0e^{-bj^{\frac1s}}. \tag{A3.6}$$

2 - Furthermore, since order-N Gauss-Legendre quadratures are exact on polynomials of order $\leqslant 2N-1$, we have, formally,

$$E_N(f)=\sum_{j=2N}^\infty c_jE_N(T_j). \tag{A3.7}$$

As was proved by A.R. Curtis and P. Rabinowitz [CP72], if N is large enough, then

$$E_N(T_j)\leqslant\pi \tag{A3.8}$$

which, by (A3.6), implies that

$$E_N(f)\leqslant\pi\sum_{j=2N}^\infty c_j\leqslant\pi b_0\sum_{j=2N}^\infty e^{-bj^{\frac1s}}. \tag{A3.9}$$

Furthermore, if $\nu_{N,s}^s := \lfloor (2N)^{\frac{1}{s}} \rfloor^s$ denotes the largest integer that is $\leqslant 2N$ and has an integer s-th root, then

$$\sum_{j=2N}^{\infty} e^{-bj^{\frac{1}{s}}} \leqslant \sum_{j=\nu_{N,s}^s}^{\infty} e^{-bj^{\frac{1}{s}}} \leqslant \sum_{k=\nu_{N,s}}^{\infty} (k^s - (k-1)^s) e^{-bk} \leqslant s \sum_{k=\nu_{N,s}}^{\infty} k^{s-1} e^{-bk}. \tag{A3.10}$$

We then estimate

$$\sum_{k=\nu_{N,s}}^{\infty} k^{s-1} e^{-bk} = \frac{d^{s-1}}{d(-b)^{s-1}} \sum_{k=\nu_{N,s}}^{\infty} e^{-bk} \leqslant (s-1)! \left(\nu_{N,s} + \frac{1}{1-e^{-b}} \right)^{s-1} \frac{e^{-b\nu_{N,s}}}{1-e^{-b}} \tag{A3.11}$$

which concludes the proof of the lemma. □

References

[CP72] A.R. Curtis, P. Rabinowitz - *On the Gaussian integration of Chebyshev polynomials*, Mathematics of Computation, Vol. 26, n. 117, p. 207-211, 1972, doi:10.1090/S0025-5718-1972-0298934-5.

[Ta87] Y. Taguchi - *Fourier coefficients of periodic functions of Gevrey classes and ultradistributions*, Yokohama Mathematical Journal, Vol. 35, p. 51-60, 1987.