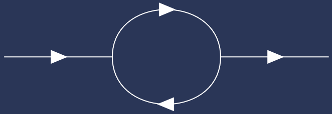
Numerical Methods for Finite Temperature Effects in Quantum Field Theory

WNPPC 2022

Siyuan Li †

February 17, 2022

†Co-supervisors: Tom Steele & Derek Harnett
Department of Physics and Engineering Physics
University of Saskatchewan



Introduction

Quantum Field Theory

- Feynman rules

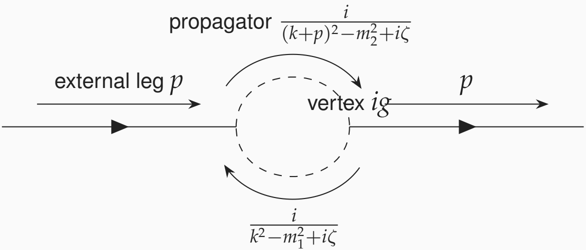


Figure 1: The one-loop self-energy Feynman diagram with scalar fields.

$$\sim g^2 \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - {m_1}^2 + i\zeta} \times \frac{1}{(k+p)^2 - {m_2}^2 + i\zeta}$$

Thermal Field Theory

The general density matrix [1]

$$\rho(\beta) = e^{-\beta\mathcal{H}},$$

The Partition function

$$Z(\beta) = \text{Tr}\,\rho(\beta) = \text{Tr}\,e^{-\beta\mathcal{H}}$$

The expectation value of an observable A

$$\langle A\rangle_\beta = Z^{-1}(\beta)\,\text{Tr}\,(\rho(\beta)\,A) = \frac{\text{Tr}\,(\,e^{-\beta\mathcal{H}}A\,)}{\text{Tr}\,e^{-\beta\mathcal{H}}}$$

The vacuum expectation value

$$\lim_{\mathcal{T}\to 0}\text{Tr}\,(\,\rho A\,) = \langle 0|\,A\,|0\rangle$$

[1] F. Gelis, Quantum Field Theory: From Basics to Modern Topics. Cambridge University Press, 2019.

Matsubara Formalism

- For free bosonic scalar fields, [2]

$$\mathcal{G}^0(\omega_n, \boldsymbol{p}) = \frac{1}{\omega_n^2 + \boldsymbol{p}^2 + m^2}$$

with the Matsubara frequency $\omega_n = 2n\pi\mathcal{T}$ being $\mathcal{T}$ dependent. Here we have $\mathcal{T} = \frac{1}{k_B \beta}$ with $k_B = 1$.

- The temporal k_0 integral is therefore discretized,

$$\int \frac{d^4k}{(2\pi)^4} \to \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}.$$

[2] F. Gelis, Quantum Field Theory: From Basics to Modern Topics. Cambridge University Press, 2019.

Thermal Field Theory

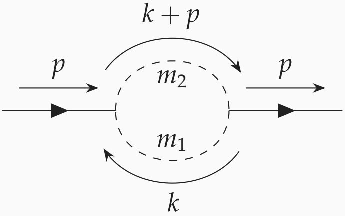


Figure 2: The one-loop self-energy Feynman diagram with scalar fields.

$$\Pi_{\mathcal{T}}(\boldsymbol{p}, p_0) = \frac{1}{2\beta} \sum_{n=-\infty}^{\infty} \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \frac{1}{\frac{4n^2\pi^2}{\beta^2} + \boldsymbol{k}^2 + {m_1}^2} \times \frac{1}{(\frac{2n\pi}{\beta} + p_0)^2 + (\boldsymbol{k} + \boldsymbol{p})^2 + {m_2}^2}$$

Methodology

Object

The object we are looking for is

$$\Pi_s = \Pi_{\mathcal{T}} - \Pi_0.$$

And the biggest difficulties we are facing from Π_s is

- the ultra-violet **divergence** in $d = 4$ spacetime (1 temporal dimension and 3 spatial dimensions) for both $\Pi_{\mathcal{T}}$ and Π_0;

$$\Pi_0(\boldsymbol{p}, p^0) = \frac{1}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + {m_1}^2} \times \frac{1}{(k+p)^2 + {m_2}^2}$$

- the application to the numerical calculation tool.

The Cut-off Method

$$\Pi_{\mathcal{T}} \approx \sum_n \frac{1}{32|n|\pi^2}, \; |n| \gg 1$$

$$\Downarrow$$

An upper limit n_{max} provides a suitable regulation method to regulate both divergent $\Pi_{\mathcal{T}}$ and Π_0.

$$\Downarrow$$

Π_s hopefully will be convergent as $n_{max} \to \infty$ and $k_{0,max} = \frac{2\pi n_{max}}{\beta} \to \infty$.

$$\Downarrow$$

the cut-off method

THE 'REVERSE' WICK ROTATION

- pySecDec: a program designed for numerical calculation of dimensionally regulated loop integrals. [3]
-

$$\Pi_{\mathcal{T}}(\boldsymbol{p}, p_0^E) = \frac{1}{2\beta} \sum_{n=-\infty}^{\infty} \underbrace{\int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \frac{1}{(\frac{2n\pi}{\beta})^2 + \boldsymbol{k}^2 + {m_1}^2} \times \frac{1}{((\frac{2n\pi}{\beta})^2 + p_0^E)^2 + (\boldsymbol{k}+\boldsymbol{p})^2 + {m_2}^2}}_{\text{This is the part we can use pySecDec to numerically evaluate.}}$$

[3] "pysecdec: A toolbox for the numerical evaluation of multi-scale integrals," arXiv:1703.09692.

The 'Reverse' Wick Rotation

$$\int \frac{d^D \boldsymbol{k}}{(2\pi)^D} \underbrace{\frac{1}{\boldsymbol{k}^2 + {\Lambda_1}^2}} \times \underbrace{\frac{1}{(\boldsymbol{k}+\boldsymbol{p})^2 + {\Lambda_2}^2}}$$

- $\Pi_{\mathcal{T}}$ expression is in Euclidean space, while pySecDec works in Minkowski space.
- pySecDec will calculate momentum in spacetime dimension while we only need to solve integral for spatial dimensions.

The 'Reverse' Wick Rotation

Define momentum k_1^m

$$k_1^m = ik_1,\ dk_1^m = i\,dk_1,\ (k_1^m)^2 = (ik_1)^2 = -k_1^2$$

Define Minkowski spacetime momentum $k^m = (k_1^m, k_2, k_3, ...k_D)$

$$k^m \cdot k^m = -\mathbf{k}^2 \tag{1}$$

Now we have an applicable form of $\Pi_{\mathcal{T}}$ for pySecDec calculation

$$\Pi_{\mathcal{T}}(\boldsymbol{p}, p_0^E) = -i\,\frac{1}{2\beta} \sum_{n=-\infty}^{\infty} \int \frac{d^3k^m}{(2\pi)^3} \frac{1}{(k^m)^2 - \Lambda_1^2} \times \frac{1}{(k^m + p^m)^2 - \Lambda_2^2},$$

where $\boldsymbol{p} = (p_1, p_2, p_3)$, $p_1^m = ip_1$, $k_1^m = ik_1$, $\Lambda_1^2 = {m_1}^2 + \omega_n^2 + i\zeta$ and $\Lambda_2^2 = m_2^2 + (p_0^E + \omega_n)^2 + i\zeta$.

The Subtraction $\Pi_s = \Pi_{\mathcal{T}} - \Pi_0$

$$
\begin{aligned}
\Pi_s &= \Pi_{\mathcal{T}} - \Pi_0 \\
&= \frac{1}{2\beta} \sum_{n=-\infty}^{\infty} I_{\mathcal{T}}(\omega_n) - \frac{1}{2} \int \frac{dk_0^E}{2\pi}\, I_0(k_0^E) \\
&\approx \frac{1}{2} \left(\sum_{n=-n_{max}}^{n_{max}} \frac{I_{\mathcal{T}}(\omega_n)}{\beta} - \sum_{n=-n_{max}}^{n_{max}-1} \int_{2\pi n/\beta}^{2\pi(n+1)/\beta} \frac{dk_0^E}{2\pi}\, I_0(k_0^E) \right)
\end{aligned}
$$

THE SUBTRACTION $\Pi_s = \Pi_{\mathcal{T}} - \Pi_0$

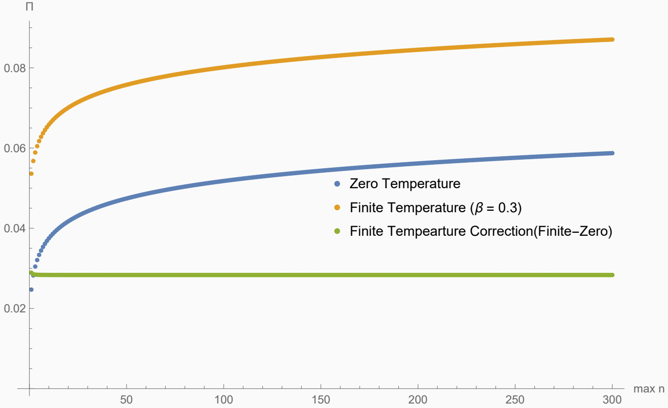


Figure 3: The numerical calculation results from pySecDec of zero-temperature correlation function Π_0 (blue), finite-temperature correlation function $\Pi_{\mathcal{T}}$ (yellow) and finite-temperature correction Π_s (green). The parameter values are $m_1 = 1.1, m_2 = 2, p_0^E = \frac{2\pi}{\beta}, \beta = 0.3, \boldsymbol{p}^2 = 1$ and maximum $|n|$ up to 300.

Convergence regarding different β values

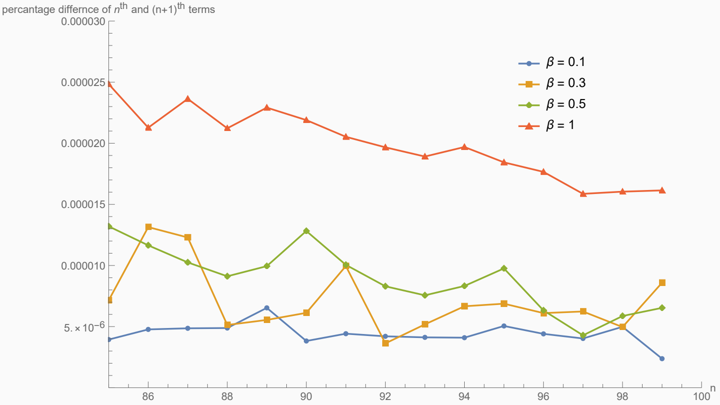


Figure 4: The percentage difference of every two adjacent terms in the summation of Π_s. The β values are shown in the legend and maximum $|n|$ up to 100.

Numerical Results

Relationship with Respect to External Momenta ($d = 4$)

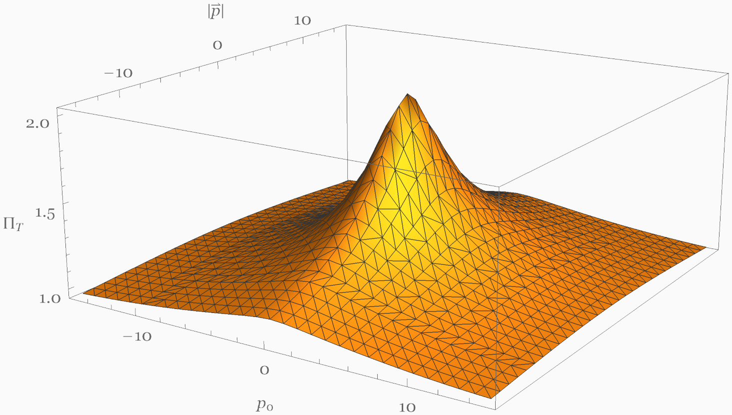


Figure 5: The effects of the external momentum p_0^E and $|\boldsymbol{p}|$ on Π_s of the one-loop self-energy topology

Relationship with Respect to Temperature $\mathcal{T}$ ($d = 4$)

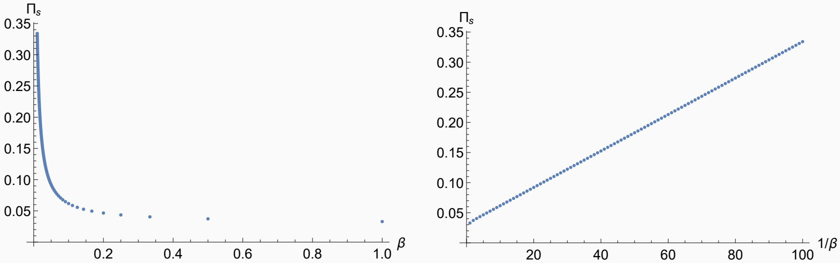


Figure 6: The plot of Π_s with respect to β (left) and $1/\beta$ (right) respectively for $d = 4$ spacetime. The slope in the right plot is approximately 0.00302586. The intercept of the right plot is approximately 0.0314978 (with parameters $m_1 = 1.1$, $m_2 = 1.2$, $p = (7, 8, 9, 6)$, $|n| = A = 100$).

Relationship with Respect to Temperature $\mathcal{T}$ ($d = 4$)

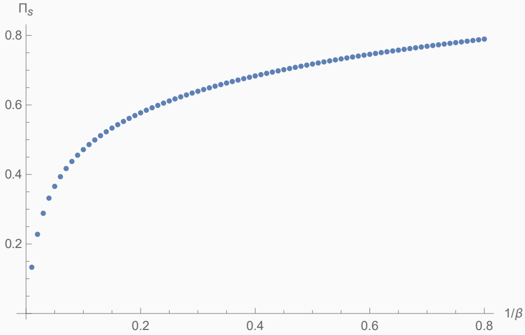


Figure 7: The plot shows the Π_s behavior at small temperature. The finite-temperature correction Π_s goes to zero as temperature goes to zero. The parameters used are the same as in Fig. 6.

Other Topologies

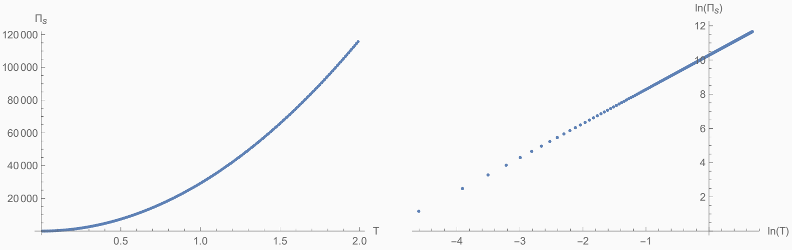


Figure 8: On the RHS is the log-log plot for the Π_s vs $\mathcal{T}$ relation. The slope on the right plot is approximately 1.99946.

Conclusions & Future Steps

Conclusions

- We developed a technique called 'reverse' Wick rotation so that we can apply $\Pi_{\mathcal{T}}$ to pySecDec for numerical evaluation;
- The cut-off method was chosen to regularize the divergence in both $\Pi_{\mathcal{T}}$ and Π_0;
- Finally we successfully calculated Π_s for one-loop self-energy topology under finite temperature in $d = 4$ spacetime.

Future Directions

- ◇ More complicated topologies can be numerically calculated;
- ◇ Alternative methodology is under development to manage the divergences from analytical approach to compare with the cut-off method.

Thank you!

Back-up Slides

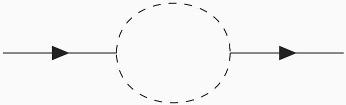
Dimension Cancellation

$$\Pi_0(\boldsymbol{p}, p^0) = \frac{\lambda^2}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1/p^2}{\left(\frac{k^2}{p^2} + \frac{{m_1}^2}{p^2}\right)} \times \frac{1/p^2}{\left(\frac{(k+p)^2}{p^2} + \frac{{m_2}^2}{p^2}\right)}$$
$$= \frac{\lambda^2}{2(2\pi)^4} \int d^4\left(\frac{k}{p}\right) \frac{1}{\left(\frac{k}{p}\right)^2 + \frac{{m_1}^2}{p^2}} \times \frac{1}{\left(\frac{k}{p} + 1\right)^2 + \frac{{m_2}^2}{p^2}}$$

Since we are using the particle physics convention of $\hbar = c = 1$, both particle masses and momenta have the dimensions of energy. All the expressions in brackets are dimensionless. So technically, what only matters for numerical benchmarking are the ratios $\frac{{m_1}^2}{p^2}$ and $\frac{{m_2}^2}{p^2}$.

pySecDec Benchmarking for Zero-Temperature Loop Integrations

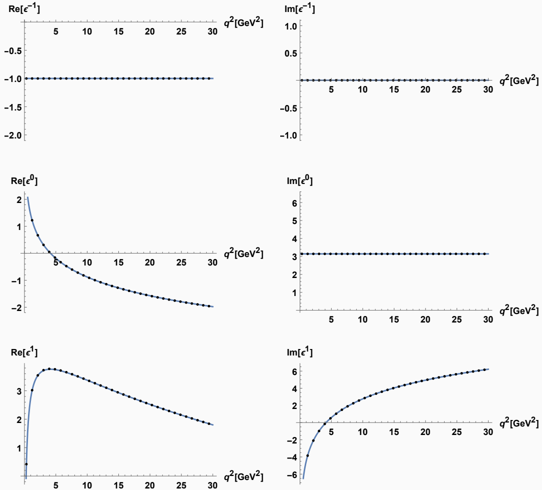
- pySecDec: a program designed for numerical calculation of dimensionally regulated loop integrals.
- One-loop self-energy topology integral (TBI).



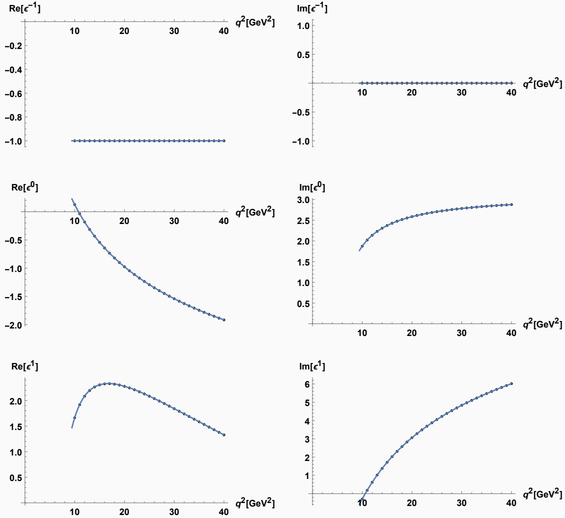
$$\text{TBI}\left[d, p^2, \{\{\nu_1, m_1\}, \{\nu_2, m_2\}\}\right] = \frac{1}{\pi^{\frac{d}{2}}} \int \frac{d^d k}{[k^2 - m_1{}^2]^{\nu_1} [(k-q)^2 - m_2{}^2]^{\nu_2}}$$

$$\text{TBI}\left[\, 4 + 2\epsilon, q^2, \{\nu_1, 0\}, \{\nu_2, 0\} \,\right] = \frac{i}{(4\pi)^2} \left[-\frac{q^2}{4\pi}\right]^{\epsilon} (q^2)^{2-\nu_1-\nu_2} \frac{\Gamma\left[2-\nu_1+\epsilon\right] \Gamma\left[2-\nu_2+\epsilon\right] \Gamma\left[\nu_1+\nu_2-2-\epsilon\right]}{\Gamma\left[\nu_1\right] \Gamma\left[\nu_2\right] \Gamma\left[4-\nu_1-\nu_2+2\epsilon\right]}$$

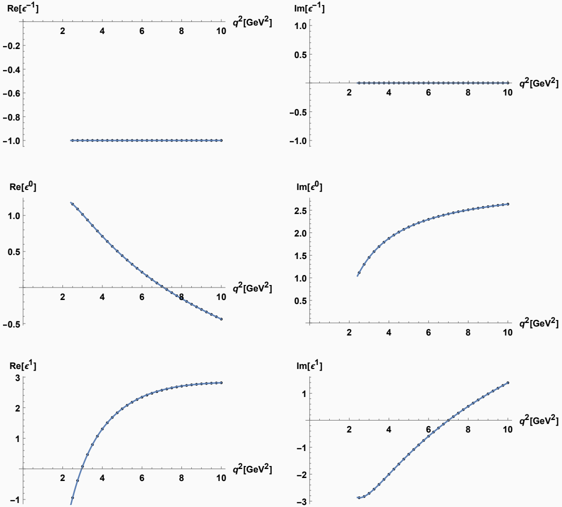
TBI Massless Integral ($m_1 = m_2 = 0\,\mathrm{GeV}, \nu_1 = \nu_2 = 1$)



TBI Massive Integral ($m_1 = m_2 = 1.27\,\mathrm{GeV}, \nu_1 = \nu_2 = 1$)



TBI Massive Integral ($m_1 = 1.27\,\mathrm{GeV},\ \mathrm{m}_2 = 0, \nu_1 = \nu_2 = 1$)



Cutting Rules

- Cutting Rules(Cutkosky rules [4]): generally used to find the imaginary part of a Feynman diagram.

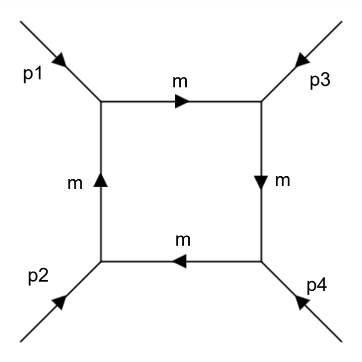


Figure 9: Four-point one-loop function topology with same internal masses

[4] M. E. Peskin, An introduction to quantum field theory. CRC press, 2018.

Cutting Rules: pySecDec Data for four-point function with $m = m_b = 4.18\ GeV$

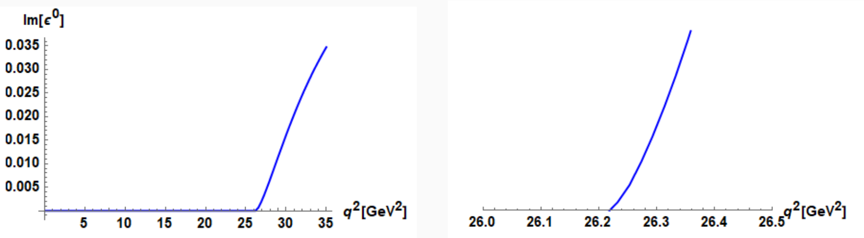
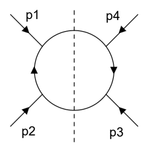
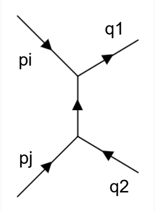


Figure 10: Above diagrams show the ϵ^0 coefficient for the four-point one-loop Feynman integral with same masses ($m = m_b = 4.18\ GeV$) along with an expanded diagram on the right hand side. The imaginary part remains zero until $q^2 \gtrapprox 26.21\ \text{GeV}^2$.

CUTTING RULES: THRESHOLD ANALYSIS

2 Im (


) $= \int d\Pi$ |


|^2

- symmetric kinematics, and with $p_4 = p_1 + p_2 + p_3$,

$$p_1^2 = p_2^2 = p_3^2 = q^2 = -\,3\,p_i \cdot p_j$$

- As all the internal lines have the same mass m,

$$q^2 > \frac{3}{2}\,m^2\,.$$

$$\frac{3}{2}\,m_b^2 = \frac{3}{2} \times (4.18\,\mathrm{GeV})^2 \approx 26.209\,\mathrm{GeV}^2.$$

Large n Behavior

$$
\begin{aligned}
\Pi_{\mathcal{T}} &= \frac{1}{2\beta}\sum_n \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\frac{1}{(\frac{4n^2\pi^2}{\beta^2}) + \boldsymbol{k}^2 + {m_1}^2} \times \frac{1}{(\frac{2n\pi}{\beta} + p_0^E)^2 + (\boldsymbol{k}+\boldsymbol{p})^2 + {m_2}^2} \\
&\approx \frac{1}{2\beta}\sum_n \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\frac{1}{(\frac{2n\pi}{\beta})^2 + \boldsymbol{k}^2} \times \frac{1}{(\frac{2n\pi}{\beta})^2 + \boldsymbol{k}^2}, \text{ for } |n| \gg 1 \\
&= \frac{1}{2\beta}\sum_n \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\frac{1}{\left(m'^2 + \boldsymbol{k}^2\right)^2}
\end{aligned}
$$

where $m' = \frac{2n\pi}{\beta}$.

LARGE n BEHAVIOR

$$\Phi(m,d,B) = \int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\frac{1}{(\mathbf{k}^2+m^2)^B} = \frac{1}{(4\pi)^{\frac{d}{2}}}\frac{\Gamma\left(B-\frac{d}{2}\right)}{\Gamma(B)}\frac{1}{(m^2)^{B-\frac{d}{2}}}$$ [5]

$$\Pi_{\mathcal{T}} \approx \frac{1}{2\beta}\sum_n \underbrace{\frac{1}{(4\pi)^{\frac{3}{2}+\epsilon}}\frac{\Gamma\left(\frac{1}{2}+\epsilon\right)}{1}}_{\text{expand } \epsilon \text{ to } \mathcal{O}(\epsilon)}\frac{1}{\left(\frac{2n\pi}{\beta}\right)^{2(1+2\epsilon)}}$$

$$\approx \frac{1}{2\beta}\sum_n \frac{\sqrt{\pi}}{(4\pi)^{\frac{3}{2}}}\frac{\beta}{2\pi\,(n^2)^{\frac{1}{2}+\epsilon}}$$

$$= \sum_n \frac{1}{32\pi^2}\frac{1}{|n|^{1+2\epsilon}}.$$

[5] M. Laine and A. Vuorinen, Basics of Thermal Field Theory. Springer International Publishing, 2016.

LARGE n BEHAVIOR

$$\Pi_{\mathcal{T}} \approx \sum_n a_n, a_n \approx \frac{1}{32|n|\pi^2}, \; |n| \gg 1.$$

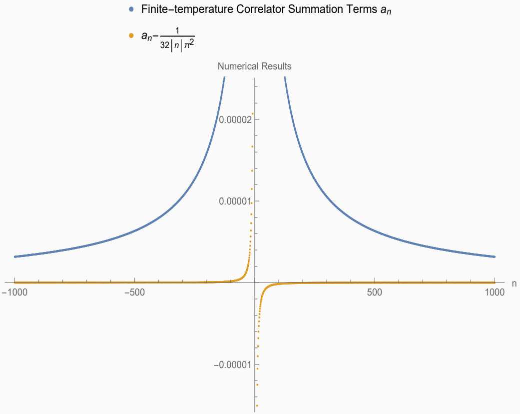


Figure 6: The pySecDec-computed $\Pi_{\mathcal{T}}$ terms $a_n \approx \frac{1}{32|n|\pi^2}$ are analyzed by calculating the difference $\Pi_{\mathcal{T}} - a_n$ as a function of n. The finite-temperature terms were calculated with the parameter values of $m_1 = m_2 = 1.1, p_0^E = \frac{2\pi}{\beta}, \beta = 0.3, \boldsymbol{p}^2 = 5$

Proof of Convergence

Define

$$C_n = A_n - A_{n+1},$$

where A_n represents individual terms from the summation in Π_s.

$$A_n = \frac{I_{\mathcal{T}}(\omega_n)}{\beta} - \int_{2\pi n/\beta}^{2\pi(n+1)/\beta} \frac{dk_0^E}{2\pi}\, I_0(k_0^E).$$

Proof of Convergence

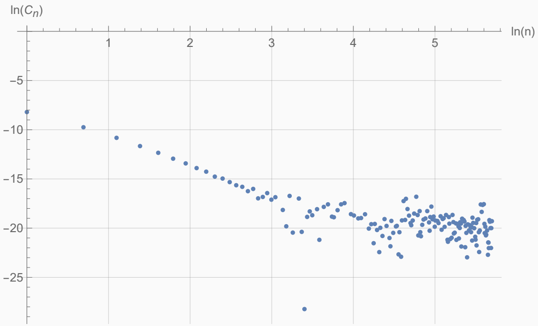


Figure 11: The plot between $\ln(C_n)$ and $\ln(n)$ shows a linear relation with a slope $-\gamma \approx -3.57$ corresponding to $C_n \approx \frac{a}{n^\gamma}$. The data in the figure was generated with the same parameters as in Fig. 3.

Proof of Convergence

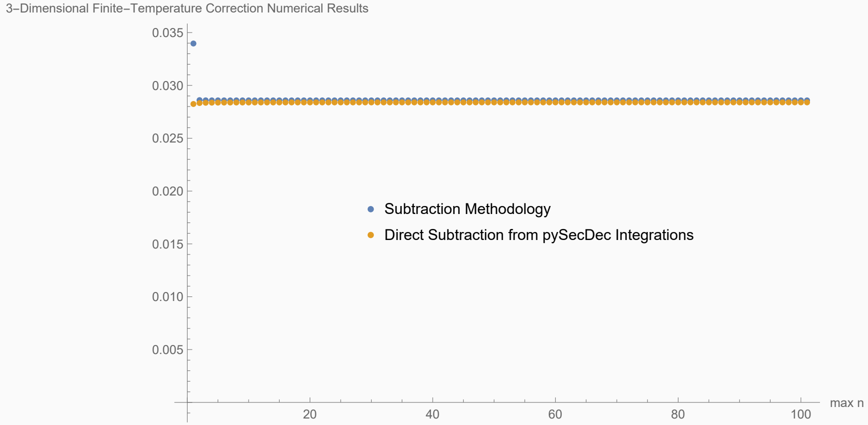
$$C_n \approx \frac{a}{n^\gamma} \Rightarrow \ln(C_n) \approx -\gamma \ln(n) + \ln(a),$$

where $\ln(a)$ is defined as the intercept in Fig. 11. Thus we find

$$C_n = A_n - A_{n+1} \approx \frac{a}{n^\gamma},$$

with $\gamma \approx 3.57 > 1$.

Methodology Benchmark for $d = 3$ Spacetime



Relationship with Respect to External Momenta ($d = 3$)

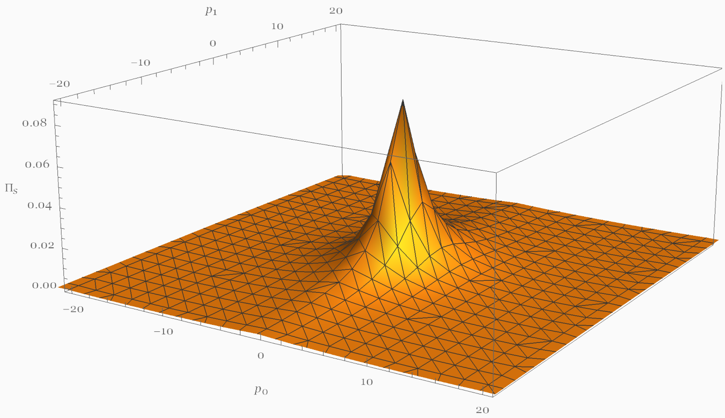


Figure 12: The effects of the external momentum on the $d = 3$ finite-temperature correction Π_s (Eq. (1)) of the one-loop self-energy topology (with same parameter values as in Fig. **??**).

Relationship with Respect to Temperature $\mathcal{T}$ ($d = 3$)

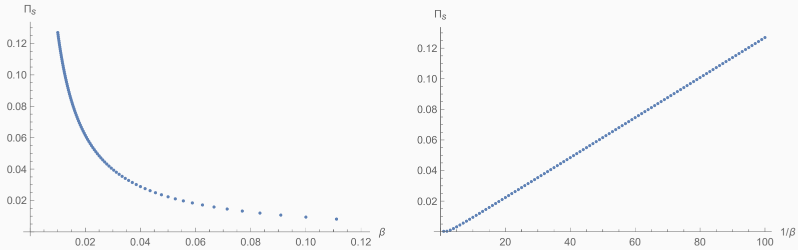


Figure 13: The plot of the finite-temperature correction Π_s as a function of β (left) and $1/\beta$ (right) at $d = 3$ spacetime. The slope on the right plot is approximately 0.00130617. The parameters used in the calculation are $m_1 = 1.1, m_2 = 1.2, p_\mu = (7, 8, 9, 0)$.

CONVERGENCE REGARDING DIFFERENT β VALUES

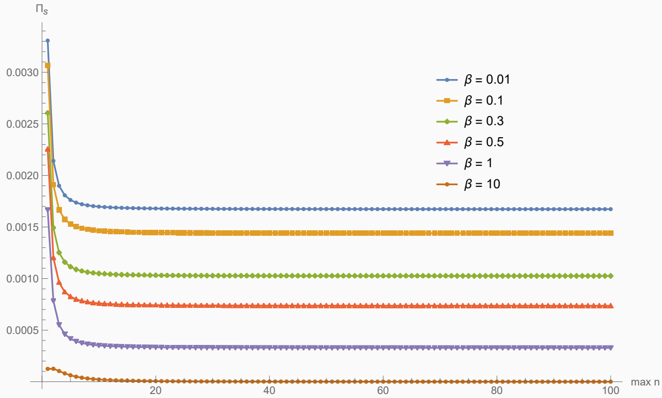


Figure 14: The numerical calculation results from pySecDec of finite-temperature correction Π_s. The β values are shown in the legend and maximum $|n|$ up to 100.

THE CONVERGENCE OF Π_s

Define $A_n = \frac{I_{\mathcal{T}}(\omega_n)}{\beta} - \int_{2\pi n/\beta}^{2\pi(n+1)/\beta} \frac{dk_0^E}{2\pi} I_0(k_0^E)$. Confirm $A_n \approx \frac{a}{n^\gamma}$.

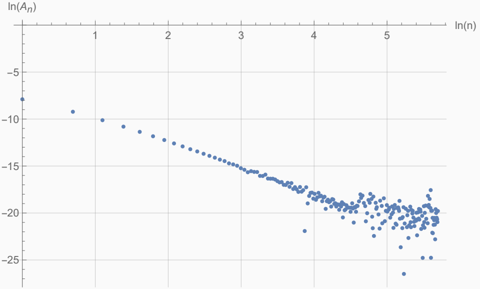


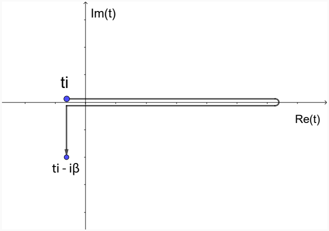
Figure 15: The plot between $\ln(A_n)$ and $\ln(n)$ shows a linear relation with a slope $-\gamma \approx -2.80$ corresponding to $A_n \approx \frac{a}{n^\gamma}$.

Matsubara Formalism

- The density operator

$$e^{-\beta\mathcal{H}} = e^{-\beta\mathcal{H}_0}\,\mathcal{U}(t_i - i\beta, t_i) = e^{-\beta\mathcal{H}_0}\,\mathsf{T}\exp\left[i\int_{t_i}^{t_i - i\beta} d^4x\mathcal{L}_I(\phi_{in}(x))\right]$$

  where $\mathcal{U}$ is the time evolution operator.
- The contour is then $\mathcal{C} = [t_i, +\infty] \cup [+\infty, t_i] \cup [t_i, t_i - i\beta]$.



Matsubara Formalism

- The quantities that describe the thermodynamics of a system in thermal equilibrium are time independent.

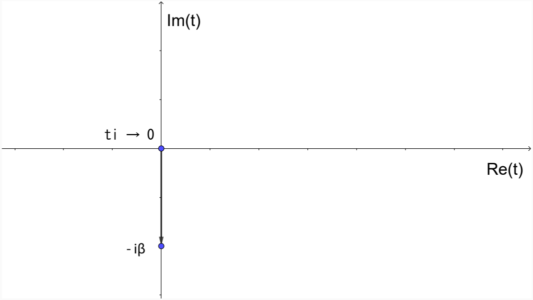


Figure 16: Simplified contour $\mathcal{C}$ of thermal time (taking initial thermal time $\rightarrow 0$).