Integration-by-parts improvement of Fermi integrals for baryon number susceptibilities at low temperature

Technical note for Thermal-FIST

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Abstract

We describe the integration-by-parts (IBP) technique used to improve the numerical evaluation of Fermi-Dirac integrals for baryon number susceptibilities χ_n^B at low temperatures in the hadron resonance gas model. The key idea is to reduce the order of the Fermi–Dirac distribution derivatives appearing in the integrand by one, replacing oscillatory or sharply peaked integrands with smoother ones that are better resolved by the existing Sommerfeld–Legendre + Laguerre quadrature scheme. We present the IBP formulas for χ_2, χ_3, and χ_4, derive the analytic $T = 0$ limits, and document the numerical improvements achieved.

Contents

1 Setup and notation

Consider a single fermion species with mass m, degeneracy g, at temperature T and chemical potential $\mu > m$ (so that the Fermi momentum $p_{\mathrm{F}} = \sqrt{\mu^2 - m^2}$ is real). The Fermi–Dirac distribution is

$$f(p) = \frac{1}{e^{(E-\mu)/T} + 1}, \qquad E = \sqrt{p^2 + m^2}. \tag{1}$$

The particle number density is

$$n = \frac{g}{2\pi^2} \int_0^\infty p^2 f(p)\, dp. \tag{2}$$

The generalized susceptibilities are the μ-derivatives of the pressure, or equivalently:

$$\chi_n \equiv \frac{\partial^n P}{\partial \mu^n} = \frac{\partial^{n-1} n}{\partial \mu^{n-1}}. \tag{3}$$

Using the identity $\partial f/\partial\mu = f(1-f)/T$, the first few susceptibilities involve

$$\chi_2 = \frac{\partial n}{\partial \mu} = \frac{g}{2\pi^2} \int_0^\infty p^2 \frac{f(1-f)}{T}\, dp, \tag{4}$$

$$\chi_3 = \frac{\partial^2 n}{\partial \mu^2} = \frac{g}{2\pi^2} \int_0^\infty p^2 \frac{f(1-f)(1-2f)}{T^2}\, dp, \tag{5}$$

$$\chi_4 = \frac{\partial^3 n}{\partial \mu^3} = \frac{g}{2\pi^2} \int_0^\infty p^2 \frac{f(1-f)\big[1-6f(1-f)\big]}{T^3}\, dp. \tag{6}$$

The numerical problem. As $T \to 0$, the factor $f(1-f)/T$ tends to $\delta(E-\mu)$, i.e. $\delta(p-p_{\mathrm{F}})/v_F$ with $v_F = p_{\mathrm{F}}/\mu$. For χ_2 the integrand is a narrow positive peak at p_{F}; for χ_3 the integrand $f(1-f)(1-2f)/T^2$ has a derivative-of-delta structure (one sign change); for χ_4 the integrand $f(1-f)[1-6f(1-f)]/T^3$ has a second-derivative-of-delta structure (two sign changes). Higher-order integrands are increasingly oscillatory and harder for fixed-order quadrature to resolve.

We use a hybrid quadrature scheme:

- **Sommerfeld–Legendre** (32 points): maps $[0,1] \to [0, p_{\mathrm{F}}]$ with adaptive concentration of quadrature nodes near the Fermi surface, controlled by $\alpha = p_{\mathrm{F}}^2/(\mu T)$.
- **Shifted Laguerre** (32 points): covers $[p_{\mathrm{F}}, \infty)$ with exponential weight.

Both sets of nodes are concentrated near p_{F}, where the Fermi–Dirac integrands peak. However, for the oscillatory integrands in χ_3 and especially χ_4, the quadrature accuracy degrades severely at low T. The IBP technique described below smooths the integrands by reducing the derivative order by one.

2 IBP identities

The core identity underlying all IBPs is

$$\frac{df}{dp} = -\frac{p}{ET} f(1-f). \tag{7}$$

This allows us to express products of f and its μ-derivatives as total p-derivatives, enabling integration by parts.

2.1 χ_2: first IBP

From eq. (7), we have

$$f(1-f) = -T\,\frac{E}{p}\,\frac{df}{dp}\,. \tag{8}$$

Therefore the χ_2 integrand becomes a total derivative:

$$p^2\,f(1-f) = -T\,p\,E\,\frac{df}{dp} = -T\,\frac{d}{dp}\big[p\,E\,f\big] + T\,\frac{d(pE)}{dp}\,f\,. \tag{9}$$

Since $d(pE)/dp = (2p^2+m^2)/E$ and the boundary term $[p\,E\,f]_0^\infty = 0$ (vanishes at $p=0$ and exponentially at $p=\infty$), integration by parts gives

$$\boxed{\int_0^\infty p^2\,f(1-f)\,dp = T\int_0^\infty \frac{2p^2+m^2}{E}\,f\,dp\,.} \tag{10}$$

The left-hand side has integrand $f(1-f)\sim\delta(p-p_{\mathrm{F}})$; the right-hand side has integrand f, the Fermi step function itself — smooth, monotonic, and trivial for quadrature.

Using eq. (10) in eq. (4):

$$\chi_2 = \frac{g}{2\pi^2}\int_0^\infty \frac{2p^2+m^2}{E}\,f\,dp\,. \tag{11}$$

2.2 χ_3: second IBP

Differentiating $f(1-f) = -T(E/p)\,df/dp$ once more with respect to μ:

$$\frac{\partial}{\partial\mu}\big[f(1-f)\big] = \frac{f(1-f)(1-2f)}{T} \quad\Rightarrow\quad f(1-f)(1-2f) = -T\,\frac{E}{p}\,\frac{d}{dp}\big[f(1-f)\big]\,. \tag{12}$$

Therefore

$$p^2\,f(1-f)(1-2f) = -T\,p\,E\,\frac{d}{dp}\big[f(1-f)\big]\,. \tag{13}$$

Integrating by parts with $[p\,E\,f(1-f)]_0^\infty = 0$ (the boundary terms vanish since $pE=0$ at $p=0$ and $f(1-f)$ decays exponentially at $p\to\infty$):

$$\boxed{\int_0^\infty p^2\,f(1-f)(1-2f)\,dp = T\int_0^\infty \frac{2p^2+m^2}{E}\,f(1-f)\,dp\,.} \tag{14}$$

The left-hand side has an integrand with one sign change (derivative-of-delta structure); the right-hand side has $f(1-f)$, a smooth non-negative peak at p_{F} — the same integrand that appeared in the *un-improved* χ_2.

Using eq. (14) in eq. (5):

$$\chi_3 = \frac{g}{2\pi^2 T}\int_0^\infty \frac{2p^2+m^2}{E}\,f(1-f)\,dp\,. \tag{15}$$

2.3 χ_4: third IBP

Similarly, differentiating $f(1-f)(1-2f)$ with respect to μ:

$$\frac{\partial}{\partial\mu}\big[f(1-f)(1-2f)\big] = \frac{f(1-f)\big[1-6f(1-f)\big]}{T} \tag{16}$$

and thus

$$f(1-f)\big[1-6f(1-f)\big] = -T\,\frac{E}{p}\,\frac{d}{dp}\big[f(1-f)(1-2f)\big]\,. \tag{17}$$

Integration by parts with $[p\,E\,f(1{-}f)(1{-}2f)]_0^\infty = 0$ gives:

$$\boxed{\int_0^\infty p^2\, f(1-f)\big[1-6f(1-f)\big]\, dp = T\int_0^\infty \frac{2p^2+m^2}{E}\, f(1-f)(1-2f)\, dp\,.} \tag{18}$$

The left-hand side has two sign changes; the right-hand side has one sign change (the same integrand as the *un-improved* χ_3).

Using eq. (18) in eq. (6):

$$\chi_4 = \frac{g}{2\pi^2 T^2}\int_0^\infty \frac{2p^2+m^2}{E}\, f(1-f)(1-2f)\, dp\,. \tag{19}$$

2.4 General pattern

The IBP has a recursive structure. Define

$$F_k(p) \equiv T\frac{\partial^k f}{\partial \mu^k}\,, \tag{20}$$

so that $F_0 = f$, $F_1 = f(1-f)$, $F_2 = f(1-f)(1-2f)/T$, etc. Then the identity $\partial f/\partial p = -(p/ET)\, F_1$ generalizes to

$$F_{k+1} = \frac{\partial F_k}{\partial \mu} = -T\,\frac{E}{p}\,\frac{\partial F_k}{\partial p}\,, \tag{21}$$

and each IBP step replaces

$$\int_0^\infty p^2\, F_{k+1}\, dp = T\int_0^\infty \frac{2p^2+m^2}{E}\, F_k\, dp\,, \tag{22}$$

provided the boundary term $[pE\,F_k]_0^\infty$ vanishes. Each step reduces the number of sign changes in the integrand by one, at the cost of introducing one additional power of T in the denominator when forming χ_n.

3 Analytic $T = 0$ limits

At $T = 0$, the Fermi–Dirac distribution becomes a step function, $f = \theta(p_\mathrm{F} - p)$, and the integrals can be evaluated analytically.

3.1 Density and equation of state

$$n\big|_{T=0} = \frac{g}{2\pi^2}\,\frac{p_\mathrm{F}^3}{3}\,, \tag{23}$$

$$P\big|_{T=0} = \frac{g}{6\pi^2}\left[\mu\, p_\mathrm{F}^3 - \tfrac{3}{4}\, p_\mathrm{F}^4\, \psi(m/p_\mathrm{F})\right], \tag{24}$$

$$\varepsilon\big|_{T=0} = \frac{g}{2\pi^2}\,\frac{p_\mathrm{F}^4}{4}\,\psi(m/p_\mathrm{F})\,, \tag{25}$$

where $\psi(x) = (1+x^2)^{1/2}(1+\frac{1}{2}x^2) - \frac{1}{2}x^4 \sinh^{-1}(1/x)$.

3.2 Susceptibilities

Using $f(1-f)/T \to \delta(p-p_\mathrm{F})\,\mu/p_\mathrm{F}$ and its derivatives, or by directly differentiating the $T=0$ density:

$$\chi_2\big|_{T=0} = \frac{dn}{d\mu}\bigg|_{T=0} = \frac{g}{2\pi^2}\,\frac{\mu\,p_\mathrm{F}}{1} = \frac{g}{2\pi^2}\,\mu\,p_\mathrm{F}\,, \tag{26}$$

$$\chi_3\big|_{T=0} = \frac{d^2n}{d\mu^2}\bigg|_{T=0} = \frac{g}{2\pi^2}\,\frac{\mu^2+p_\mathrm{F}^2}{p_\mathrm{F}}\,, \tag{27}$$

$$\chi_4\big|_{T=0} = \frac{d^3n}{d\mu^3}\bigg|_{T=0} = \frac{g}{2\pi^2}\,\frac{\mu\,(3p_\mathrm{F}^2-\mu^2)}{p_\mathrm{F}^3}\,. \tag{28}$$

These analytic values serve as reference for assessing the numerical accuracy at finite but small T.

4 Decomposition into below- and above-p_F contributions

The quadrature scheme splits every integral at the Fermi momentum p_F:

$$\int_0^\infty (\ldots)\,dp = \underbrace{\int_0^{p_\mathrm{F}} (\ldots)\,dp}_{\text{below } p_\mathrm{F}} + \underbrace{\int_{p_\mathrm{F}}^\infty (\ldots)\,dp}_{\text{above } p_\mathrm{F}}\,. \tag{29}$$

Since $f \to \theta(p_\mathrm{F}-p)$ as $T \to 0$, the above-p_F part vanishes exponentially, while the below-p_F part approaches a T-independent limit. We now show how this split interacts with the IBP integrands of each susceptibility.

4.1 χ_2: the $T=0$ value emerges explicitly

The IBP formula for χ_2 (eq. (10)) gives

$$T\,\chi_2 = \frac{g}{2\pi^2}\int_0^\infty \frac{2p^2+m^2}{E}\,f\,dp\,. \tag{30}$$

The integrand involves f — the Fermi step function. Below p_F we write $f = 1-(1-f)$, obtaining

$$\int_0^{p_\mathrm{F}} \frac{2p^2+m^2}{E}\,f\,dp = \underbrace{\int_0^{p_\mathrm{F}} \frac{2p^2+m^2}{E}\,dp}_{=\,\mu\,p_\mathrm{F}} - \int_0^{p_\mathrm{F}} \frac{2p^2+m^2}{E}\,(1-f)\,dp\,. \tag{31}$$

The first integral is the *exact* $T=0$ contribution and can be evaluated analytically:

$$\int_0^{p_\mathrm{F}} \frac{2p^2+m^2}{E}\,dp = \int_0^{p_\mathrm{F}} \left(2E - \frac{m^2}{E}\right)dp = \big[p\,E\big]_0^{p_\mathrm{F}} = p_\mathrm{F}\cdot\mu = \mu\,p_\mathrm{F}\,, \tag{32}$$

where we used $d(pE)/dp = (2p^2+m^2)/E$ and the boundary values $p\,E|_{p=p_\mathrm{F}} = p_\mathrm{F}\,\mu$, $p\,E|_{p=0} = 0$.

The remaining terms are thermal corrections that vanish as $T \to 0$:

- $-\int_0^{p_\mathrm{F}} \frac{2p^2+m^2}{E}\,(1-f)\,dp$: the "hole" contribution below p_F. At $T=0$, $1-f=0$ for $p<p_\mathrm{F}$, so this integral vanishes. At finite T, $1-f$ is exponentially small except near p_F, contributing $O(T^2)$.

- $+\int_{p_\mathrm{F}}^{\infty} \frac{2p^2+m^2}{E} f\,dp$: the "tail" contribution above p_F. Again $f \to 0$ for $p > p_\mathrm{F}$ as $T \to 0$, giving $O(T^2)$.

The code therefore computes

$$T\,\chi_2 = \frac{g}{2\pi^2}\,T\,\big(\underbrace{\mu\,p_\mathrm{F}}_{\text{ret2}} + \underbrace{\Delta_\mathrm{th}}_{\text{ret1}}\big)\,, \tag{33}$$

where ret2 $= \mu\,p_\mathrm{F}$ is the analytic $T = 0$ value of χ_2 (in natural units, up to the $g/2\pi^2$ prefactor) and

$$\Delta_\mathrm{th} = -\int_0^{p_\mathrm{F}} \frac{2p^2+m^2}{E}\,(1-f)\,dp + \int_{p_\mathrm{F}}^{\infty} \frac{2p^2+m^2}{E}\,f\,dp \tag{34}$$

is the thermal correction, which tends to zero as $T \to 0$.

Key point. The analytic extraction for χ_2 is *not* a numerical convenience — it is a structural consequence of the IBP. The IBP replaces the sharply peaked integrand $f(1-f)$ by the step-function-like f, which *naturally* splits into a filled Fermi sea (yielding the exact $T = 0$ answer) plus corrections from particles and holes near the Fermi surface.

4.2 χ_3: peaked integrand, no natural $T = 0$ split

The IBP formula for χ_3 (eq. (14)) gives

$$T^2\,\chi_3 = \frac{g}{2\pi^2}\,T \int_0^{\infty} \frac{2p^2+m^2}{E}\,f(1-f)\,dp\,. \tag{35}$$

The integrand $f(1-f)$ is a smooth, non-negative peak localized within $\sim T$ of p_F. Unlike the χ_2 case, $f(1-f)$ vanishes at $T = 0$ for all p (both below and above p_F), so there is no filled-Fermi-sea piece to extract directly from the integrand.

Instead, the integral scales as $\sim T$ for small T:

$$\int_0^{\infty} \frac{2p^2+m^2}{E}\,f(1-f)\,dp \xrightarrow{T\to 0} T\,\frac{\mu^2+p_\mathrm{F}^2}{p_\mathrm{F}}\,, \tag{36}$$

because $f(1-f)/T \to \delta(p-p_\mathrm{F})\,\mu/p_\mathrm{F}$. Therefore $\chi_3 = \mathrm{quad}/T \to (\mu^2+p_\mathrm{F}^2)/p_\mathrm{F}$ as $T \to 0$.

For the $T = 0$ extraction, the code computes

$$T^2\,\chi_3 = \frac{g}{2\pi^2}\,T^2\big(\underbrace{(\mu^2+p_\mathrm{F}^2)/p_\mathrm{F}}_{\text{ret2}} + \underbrace{\mathrm{quad}/T - (\mu^2+p_\mathrm{F}^2)/p_\mathrm{F}}_{\text{ret1}}\big)\,. \tag{37}$$

Here ret2 is the known $T = 0$ limit and ret1 is the thermal correction. Unlike the χ_2 case, ret2 does not emerge organically from splitting the integral at p_F — it is an independently computed constant that is subtracted. This decomposition is mathematically equivalent to the direct computation ($T^2 \times \text{value}/T^2$ round-trips losslessly in IEEE double), but it makes the $T \to 0$ behavior transparent.

4.3 χ_4: sign-changing integrand

The IBP formula for χ_4 (eq. (18)) gives

$$T^3\,\chi_4 = \frac{g}{2\pi^2}\,T \int_0^{\infty} \frac{2p^2+m^2}{E}\,f(1-f)(1-2f)\,dp\,. \tag{38}$$

The integrand $f(1-f)(1-2f)$ is localized near p_F and changes sign once (positive for $p < p_\mathrm{F}$, negative for $p > p_\mathrm{F}$, since $1-2f$ flips sign at $E = \mu$). Like χ_3, the integrand vanishes everywhere at $T = 0$, and the integral scales as $\sim T^2$:

$$\int_0^{\infty} \frac{2p^2+m^2}{E}\,f(1-f)(1-2f)\,dp \xrightarrow{T\to 0} T^2\,\frac{\mu(3p_\mathrm{F}^2-\mu^2)}{p_\mathrm{F}^3}\,. \tag{39}$$

The code uses the same extraction structure:

$$T^3\,\chi_4 = \frac{g}{2\pi^2}\,T^3\big(\underbrace{\mu(3p_{\mathrm{F}}^2-\mu^2)/p_{\mathrm{F}}^3}_{\text{ret2}} + \underbrace{\text{quad}/T^2 - \mu(3p_{\mathrm{F}}^2-\mu^2)/p_{\mathrm{F}}^3}_{\text{ret1}}\big)\,. \tag{40}$$

Because $f(1-f)(1-2f)$ has one sign change, the quadrature accuracy is intermediate between χ_2 (no sign changes, excellent) and the un-improved χ_4 (two sign changes, catastrophic).

4.4 Comparison of the three cases

The qualitative difference between χ_2 and $\chi_{3,4}$ is summarized in the following table:

	χ_2	χ_3	χ_4
IBP integrand	f	$f(1-f)$	$f(1-f)(1-2f)$
Sign changes	0	0	1
$T \to 0$ behavior of integrand	$\to \theta(p_{\mathrm{F}}-p)$	$\to 0$ (peak $\sim T$)	$\to 0$ (peak $\sim T$)
T=0 from integral splitting?	**Yes**	No	No
How T=0 enters	$\int_0^{p_{\mathrm{F}}} \frac{2p^2+m^2}{E}\,dp = \mu p_{\mathrm{F}}$	quad$/T \to$ const	quad$/T^2 \to$ const

For χ_2, the IBP is special: the integrand f has a non-vanishing $T=0$ limit (the filled Fermi sea), and splitting $f = 1-(1-f)$ below p_{F} yields the analytic answer *organically.* For χ_3 and χ_4, the integrands are purely thermal ($\to 0$ everywhere as $T \to 0$), so the $T=0$ values emerge only through the scaling of the integral with powers of T, and the analytic extraction is a separate subtraction rather than a structural decomposition.

5 Implementation details

5.1 Quadrature scheme

The integration domain $[0,\infty)$ is split at the Fermi momentum p_{F}:

Below p_{F}: Sommerfeld–Legendre quadrature. A nonlinear mapping $s \in [0,1] \to p \in [0, p_{\mathrm{F}}]$ concentrates quadrature nodes near the Fermi surface:

$$p(s) = p_{\mathrm{F}}\left(1 - \frac{u(s)}{\alpha}\right), \qquad u(s) = -\ln\big(1-\beta\,(1-s)\big), \qquad \alpha = \frac{p_{\mathrm{F}}^2}{\mu T}, \qquad \beta = 1 - e^{-\alpha}\,. \tag{41}$$

This is applied with 32-point Gauss–Legendre nodes and weights on $[0,1]$. For $\alpha \ll 1$ (i.e. $T \gg p_{\mathrm{F}}^2/\mu$, or equivalently $T \gg$ Fermi energy), the mapping reduces to uniform: $p = s\,p_{\mathrm{F}}$.

Above p_{F}: shifted Laguerre quadrature. The substitution $p = p_{\mathrm{F}} + T\,t$ transforms the Laguerre integration variable $t \in [0,\infty)$ with 32-point Gauss–Laguerre nodes and weights. The Jacobian $dp = T\,dt$ contributes a factor T.

5.2 Below-p_{F} forms

For $p < p_{\mathrm{F}}$, we have $E < \mu$ so $x = (E - \mu)/T < 0$. The Fermi–Dirac products are evaluated using e^x (which is < 1):

$$f = \frac{1}{e^x + 1}\,, \tag{42}$$

$$f(1-f) = \frac{e^x}{(1 + e^x)^2}\,, \tag{43}$$

$$f(1-f)(1-2f) = \frac{e^x}{(1 + e^x)^2}\left(1 - \frac{2}{e^x + 1}\right) = \frac{e^x(e^x - 1)}{(1 + e^x)^3}\,. \tag{44}$$

These forms are numerically stable for all $x < 0$.

For χ_2, the code computes

$$-\int_0^{p_{\mathrm{F}}} \frac{2p^2 + m^2}{E}\,\frac{1}{e^{-(E-\mu)/T} + 1}\,dp\,, \tag{45}$$

where the negative sign and e^{-x} in the denominator implement the "hole" integrand $-(1-f) = -(e^{-x}/(1+e^{-x})) = -1/(e^{-(E-\mu)/T}+1)$. This equals $-\int_0^{p_{\mathrm{F}}}(2p^2+m^2)/E\cdot(1-f)\,dp$, which when combined with the analytic $\mu\,p_{\mathrm{F}}$ from $\int_0^{p_{\mathrm{F}}}(2p^2+m^2)/E\,dp$ gives the total below-p_{F} contribution.

5.3 Above-p_{F} forms

For $p > p_{\mathrm{F}}$, we have $x = (E - \mu)/T > 0$. The substitution $p = p_{\mathrm{F}} + T\,t$ maps the integration to Laguerre variables $t \in [0, \infty)$, and the Fermi–Dirac products are evaluated using e^{-x} (which is < 1):

$$f = \frac{e^{-x}}{1 + e^{-x}}\,, \tag{46}$$

$$f(1-f) = \frac{e^{-x}}{(1 + e^{-x})^2}\,, \tag{47}$$

$$f(1-f)(1-2f) = \frac{e^{-x}(1 - e^{-x})}{(1 + e^{-x})^3}\,. \tag{48}$$

In terms of the scaled variable t, the momentum is $p = T\,t$, the energy-over-T is $E/T = \sqrt{t^2 + (m/T)^2}$, and $x = E/T - \mu/T$. The kinematic factor becomes

$$\frac{2p^2 + m^2}{E}\,dp = T^2\,\frac{2t^2 + (m/T)^2}{E/T}\,dt\,. \tag{49}$$

The extra factor of T^2 (one from $dp = T\,dt$, one from $2p^2/E = 2T^2t^2/(ET)$, but the m^2/E term contributes less) appears in the code as the explicit `T*T` multiplying the Laguerre contribution.

5.4 Analytic $T = 0$ extraction

The code stores each susceptibility in the form

$$T^k\,\chi_{k+1} = \frac{g}{2\pi^2}\,T^k\big(\underbrace{\chi^{(0)}_{k+1}}_{\text{ret2}} + \underbrace{\Delta\chi_{k+1}}_{\text{ret1}}\big)\,, \tag{50}$$

where $\chi^{(0)}_{k+1}$ is the analytic $T = 0$ value from section 3 and $\Delta\chi_{k+1} = \text{quad}/T^k - \chi^{(0)}_{k+1}$ is the thermal correction.

- For χ_2 ($k = 1$): the extraction is structural. The below-p_F quadrature computes the hole contribution $-\int_0^{p_\mathrm{F}}(2p^2+m^2)/E\cdot(1-f)\,dp$, the above-$p_\mathrm{F}$ quadrature computes the tail $+\int_{p_\mathrm{F}}^{\infty}(2p^2+m^2)/E\cdot f\,dp$, and $\mathrm{ret2} = \mu\, p_\mathrm{F}$ is the exact Fermi-sea integral. The sum $\mathrm{ret1}+\mathrm{ret2}$ equals the full χ_2 value to machine precision.
- For χ_3 ($k = 2$): both quadratures compute $\int(2p^2+m^2)/E\cdot f(1-f)\,dp$ directly (no $f = 1-(1-f)$ decomposition, since $f(1-f)\to 0$ below p_F). The analytic value $\mathrm{ret2} = (\mu^2+p_\mathrm{F}^2)/p_\mathrm{F}$ is subtracted after dividing the total quadrature by T.
- For χ_4 ($k = 3$): similarly, both quadratures compute $\int(2p^2+m^2)/E\cdot f(1-f)(1-2f)\,dp$ directly, and $\mathrm{ret2} = \mu(3p_\mathrm{F}^2-\mu^2)/p_\mathrm{F}^3$ is subtracted after dividing by T^2.

Since $T^k \times \mathrm{value}/T^k$ round-trips without precision loss in IEEE-754 double arithmetic (no overflow or underflow for $T \gtrsim 10^{-6}$ GeV), this decomposition is numerically equivalent to the direct computation in all cases.

5.5 Summary of implemented formulas

The code computes $T^k\, d^kn/d\mu^k$ for $k = 1, 2, 3$ using the IBP-improved integrands:

Quantity	**Code returns**	**IBP integrand**	T=0 **value of** $d^kn/d\mu^k$
$\chi_2 = dn/d\mu$	$T\,dn/d\mu$	$(2p^2+m^2)/E\cdot f$	$\mu\, p_\mathrm{F}$
$\chi_3 = d^2n/d\mu^2$	$T^2\,d^2n/d\mu^2$	$(2p^2+m^2)/E\cdot f(1-f)$	$(\mu^2+p_\mathrm{F}^2)/p_\mathrm{F}$
$\chi_4 = d^3n/d\mu^3$	$T^3\,d^3n/d\mu^3$	$(2p^2+m^2)/E\cdot f(1-f)(1-2f)$	$\mu(3p_\mathrm{F}^2-\mu^2)/p_\mathrm{F}^3$

All integrands include the common prefactor $g/(2\pi^2)$ and an overall factor of T from the IBP (absorbed into the T^k prefactor). The density (n, $k = 0$), pressure (P), and energy density (ε) do not use IBP — their integrands (p^2f, p^4f/E, p^2Ef) are already smooth.

6 Numerical results

We test the IBP improvements using the `ZeroTemperatureComparison` example at $\mu_B = 1.2$ GeV with the PDG2025 particle list, comparing the Ideal HRG, excluded-volume diagonal (EV), quantum van der Waals (QvdW), and real gas (CS+VDW) models. All models use quantum statistics with 32+32 quadrature points.

Tables 1 and 2 show relative deviations of the finite-T results from the exact $T = 0$ values.

Table 1: Relative deviation $(\chi_3(T)-\chi_3(0))/\chi_3(0)$ at various temperatures.

	Old (Laguerre only)		**New (IBP)**	
Model	T=0.001 MeV	T=1 MeV	T=0.001 MeV	T=1 MeV
Ideal HRG	−1.000	−1.000	-1.4×10^{-4}	4.3×10^{-2}
EV-Diagonal	0.294	0.294	3.5×10^{-9}	-1.9×10^{-5}
QvdW	0.202	0.202	2.9×10^{-9}	2.1×10^{-4}
RealGas (CS+VDW)	0.879	0.879	2.4×10^{-8}	-3.6×10^{-4}

Table 2: Relative deviation $(\chi_4(T) - \chi_4(0))/\chi_4(0)$ at various temperatures.

	Old (Laguerre only)		**New (IBP)**	
Model	T=0.001 MeV	T=1 MeV	T=0.001 MeV	T=1 MeV
Ideal HRG	-1.000	-1.000	1.46	-8.7×10^{-2}
EV-Diagonal	0.846	0.846	1.6×10^{-4}	9.7×10^{-5}
QvdW	0.505	0.505	6.8×10^{-5}	3.3×10^{-4}
RealGas (CS+VDW)	3.905	3.904	1.7×10^{-3}	4.2×10^{-4}

Key observations.

1. χ_3 **(one IBP step):** The old code produced 20–100% errors for all models below $T \sim 1\,\mathrm{MeV}$, with the Ideal HRG returning essentially zero (the Laguerre-only quadrature completely misses the Fermi surface peak). After IBP, the integrand $f(1-f)$ is a smooth, non-negative peak, and the errors drop to 10^{-9}–10^{-4} at $T = 0.001\,\mathrm{MeV}$.

2. χ_4 **(one IBP step):** The old code had 50–390% errors. After IBP, the integrand $f(1-f)(1-2f)$ still has one sign change, so the improvement is less dramatic but still substantial: errors drop to 10^{-5}–10^{-3} for interacting models. The Ideal HRG at $T = 0.001\,\mathrm{MeV}$ remains challenging (146% error) because many species with large Fermi momenta contribute, and the sign-changing integrand is harder to resolve per species. By $T = 0.1\,\mathrm{MeV}$ the Ideal HRG error is already below 0.4%.

3. **The old errors are flat in T:** For the interacting models with the old code, the relative deviations are essentially constant from $T = 0.001\,\mathrm{MeV}$ to $T = 0.1\,\mathrm{MeV}$. This confirms the errors are systematic quadrature failures (the Laguerre nodes do not resolve the Fermi surface), not physical effects.

4. **A second IBP for χ_4 is not possible.** One might attempt to apply the IBP once more to replace $f(1-f)(1-2f)$ with $f(1-f)$. However, the boundary term $[pE \cdot f(1-f)]_0^\infty$ does vanish, but the resulting integrand involves $d[(2p^2+m^2)/E]/dp = p(p^2 + 2m^2)/E^3$, which when combined with $pE \cdot f(1-f)$ produces terms proportional to $(2p^2+m^2)/p$ that diverge at $p = 0$. This makes the second IBP inapplicable.

7 Summary

The IBP improvement consists of one integration-by-parts step for each susceptibility χ_n ($n \geq 2$), using the identity

$$\int_0^\infty p^2\, F_{k+1}(p)\, dp = T \int_0^\infty \frac{2p^2 + m^2}{E}\, F_k(p)\, dp\,, \tag{51}$$

where $F_k = T\, \partial^k f/\partial\mu^k$. Each step replaces an integrand with k sign changes by one with $k-1$ sign changes, dramatically improving quadrature convergence at low T. The improvement is most pronounced for χ_3 (from $\sim 100\%$ to $\sim 10^{-9}$ relative error) and significant for χ_4 (from $\sim 400\%$ to $\sim 10^{-3}$ for interacting models).

For χ_2, the IBP was already implemented earlier and replaces the $f(1-f)$ peak by the smooth Fermi step f, yielding excellent precision at all temperatures.