

# Equation of State in Partial Chemical Equilibrium

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Here are notes detailing everything I think you'd ever need to know (and likely more) about the PCE EoS that I have been using. Section 1 exhaustively details the construction of the equation of state. Section 2 explains how the equation of state is evolved during hydrodynamics with a quark fugacity factor. Section 3 explains how we treat viscosities. All of these sections assume that a single quark fugacity describes all flavors, and Section 4 outlines how separate light and strange evolution would be implemented. Finally, Section 5 is mainly plots of all thermodynamic variables in the PCE equation of state.

## 1 Construction of the Equation of State

We define the equation of state by calculating the pressure  $P$  and energy density  $\varepsilon$  as functions of the temperature  $T$  and a quark fugacity  $\gamma_q$ , as explained in Section 1.1. This is sufficient to define the EoS, although we additionally calculate the entropy density  $s$  and speed of sound  $c_s^2$  in Sections 1.2 and 1.3, respectively, as hydrodynamics requires these quantities.

### 1.1 Pressure and Energy Density

#### 1.1.1 High Temperature

Ideally, we would hope to calculate the non-equilibrium EoS with lattice QCD essentially the same way as in equilibrium. However, due to the numerical sign problem, such a calculation is thus far impractical, and lattice studies of equilibration have largely been limited to Taylor expansions near zero chemical potential. Instead, we adopt an approach based on that proposed in [1] which interpolates between two equilibrium lattice calculations: one in (2+1)-flavor QCD [2], and one in pure SU(3) gauge theory [3]. We assume that quarks and antiquarks have equal densities characterized by the quark fugacity  $\gamma_q$ , which linearly interpolates the pressure and energy density of the two lattice equations of state in the following way:

$$\frac{P}{T^4}(T, \gamma_q) = \gamma_q \frac{P_3}{T^4} \left( T \frac{T_3}{T_c(\gamma_q)} \right) + (1 - \gamma_q) \frac{P_0}{T^4} \left( T \frac{T_0}{T_c(\gamma_q)} \right), \quad (1)$$

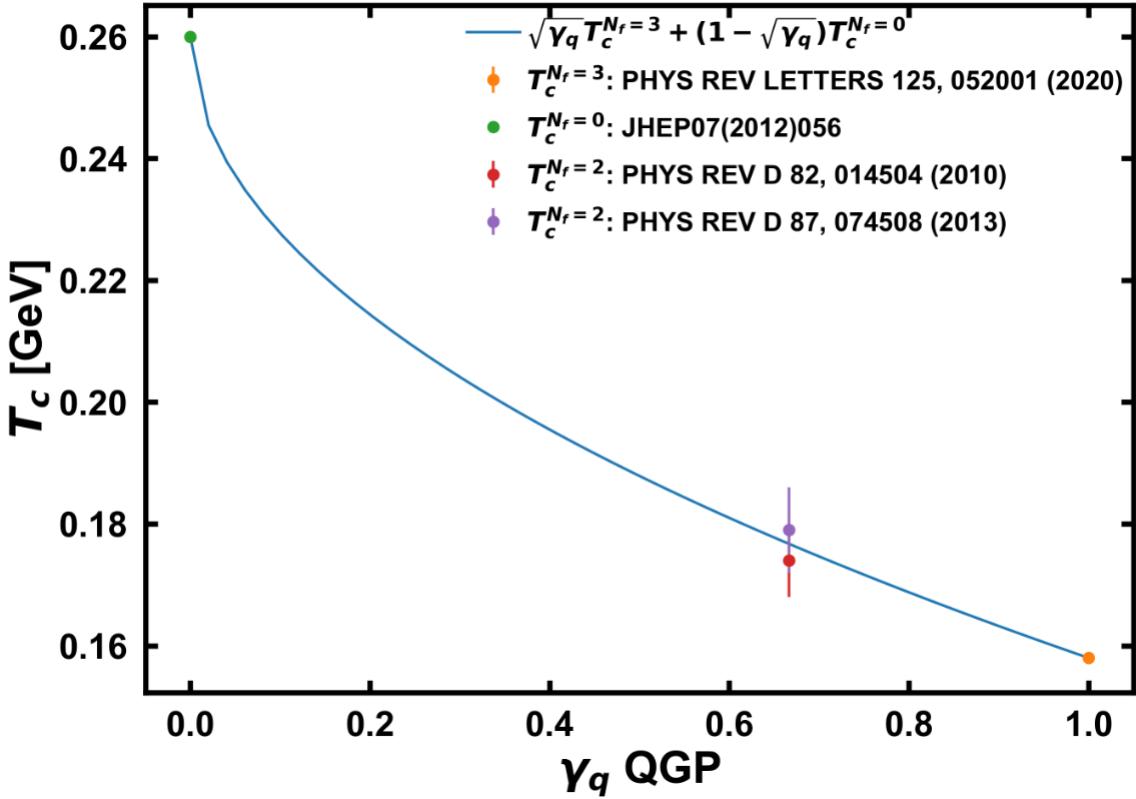
$$\frac{\varepsilon}{T^4}(T, \gamma_q) = \gamma_q \frac{\varepsilon_3}{T^4} \left( T \frac{T_3}{T_c(\gamma_q)} \right) + (1 - \gamma_q) \frac{\varepsilon_0}{T^4} \left( T \frac{T_0}{T_c(\gamma_q)} \right), \quad (2)$$

where  $P_3$ ,  $\varepsilon_3$ , and  $T_3$  are respectively the pressure, energy density, and critical temperature of the full QCD equation of state, and  $P_0$ ,  $\varepsilon_0$ , and  $T_0$  are the corresponding quantities for the pure glue equation of state. Note that at  $\gamma_q = 1$ , we recover exactly the (2+1)-flavor QCD equation of state, and at  $\gamma_q = 0$ , we recover exactly the gluonic equation of state.

As there is known to be a first order phase transition in  $N_f = 0$  at  $T_0 \approx 260$  MeV, as opposed to a crossover in  $N_f = 3$  at  $T_3 \approx 158$  MeV, simply interpolating between  $\frac{P_3}{T^4}(T)$  and  $\frac{P_0}{T^4}(T)$  would cause the system to experience separate transitions at each critical temperature for any  $0 < \gamma_q < 1$ . To avoid this, we have rescaled them according to a fugacity-dependent critical temperature  $T_c(\gamma_q)$  so that there is only ever one transition at a given fugacity.  $T_c(\gamma_q)$  is defined as

$$T_c(\gamma_q) = \sqrt{\gamma_q} T_3 + (1 - \sqrt{\gamma_q}) T_0. \quad (3)$$

This critical temperature is constructed such that it smoothly interpolates between  $T_0$  and  $T_3$  while passing through the  $N_f = 2$  critical temperature at  $\gamma_q = 2/3$  as the only applicable estimate we can extract from lattice QCD for intermediate fugacities. Figure 1 plots the result.



**Figure 1:**  $T_c(T, \gamma_q)$  compared to the critical temperatures for  $N_f = 0$ ,  $N_f = 2$ , and  $N_f = 3$  lattice results.

Note that with this temperature rescaling, the actual pressure  $P(T, \gamma_q)$  and energy density  $\varepsilon(T, \gamma_q)$  take the forms

$$P(T, \gamma_q) = \gamma_q \left( \frac{T_c(\gamma_q)}{T_3} \right)^4 P_3 \left( T \frac{T_3}{T_c(\gamma_q)} \right) + (1 - \gamma_q) \left( \frac{T_c(\gamma_q)}{T_0} \right)^4 P_0 \left( T \frac{T_0}{T_c(\gamma_q)} \right). \quad (4)$$

$$\varepsilon(T, \gamma_q) = \gamma_q \left( \frac{T_c(\gamma_q)}{T_3} \right)^4 \varepsilon_3 \left( T \frac{T_3}{T_c(\gamma_q)} \right) + (1 - \gamma_q) \left( \frac{T_c(\gamma_q)}{T_0} \right)^4 \varepsilon_0 \left( T \frac{T_0}{T_c(\gamma_q)} \right), \quad (5)$$

### 1.1.2 Low Temperature

Conventionally, the lattice equation of state at high temperature is matched to a hadron resonance gas equation of state at low temperature. We do the same here, only with modifications to the hadron distribution functions to account for non-zero quark chemical potential. This is done within the frzout particlization model [4].

The hadron resonance gas energy density and pressure are calculated as:

$$\epsilon = \sum_i g_i \int \frac{d^3 p}{(2\pi)^3} E_p f_i(p) \quad (6)$$

$$P = \sum_i g_i \int \frac{d^3 p}{(2\pi)^3} \frac{p^2}{3E_p} f_i(p), \quad (7)$$

where  $i$  denotes the hadron species,  $g_i$  and  $f_i$  are the respective degeneracy and distribution function for each species, and  $E_p = \sqrt{p^2 + m_i^2}$  is the individual hadron energy. In equilibrium, mesons are described by a Bose-Einstein distribution and baryons by a Fermi-Dirac distribution. In chemical non-equilibrium, the distribution functions can be modified to take the form

$$f_i(T, \lambda_i) = \frac{1}{\lambda_i^{-1} e^{E_p/T} \pm 1}, \quad (8)$$

where  $\lambda_i$  is a species-specific fugacity factor distinct from the  $\gamma_q$  used in the high temperature EoS.

In the simple case of symmetric quark flavors (see Section 4 for more on strangeness), we define

$$\lambda_{\text{meson}} = 0.85\gamma_q + 0.15 \quad (9)$$

$$\lambda_{\text{baryon}} = \lambda_{\text{meson}}^{3/2}, \quad (10)$$

where the admittedly ad hoc definition of  $\lambda_{\text{meson}}$  is defined such that all thermodynamic variables are continuous and differentiable over the transition region. The relation between  $\lambda_{\text{baryon}}$  and  $\lambda_{\text{meson}}$  follows simply from baryons having three (anti)quarks and mesons having two.

This low temperature result for  $\varepsilon(T, \gamma_q)$  and  $P(T, \gamma_q)$  must be matched to the high temperature values, which conventionally is done over a crossover range of  $T \sim 160 - 200$  MeV. We do the same, using Krogh interpolation, only for a fugacity-dependent temperature range defined as  $(T_c(\gamma_q) + 0.005 \text{ MeV}, T_c(\gamma_q) + (0.01 + 0.1\gamma_q) \text{ MeV})$ .

## 1.2 Entropy Density

Calculating the entropy density is not trivial, but it can be done in a straightforward manner using basic thermodynamics. Eq. 18 is the result.

Using only the fundamental thermodynamic relation

$$dU = TdS - PdV + \mu dN \quad (11)$$

and considering only the number of (anti)quarks  $N_q$ , we get

$$\varepsilon = Ts - P + \mu n_q. \quad (12)$$

Note that in equilibrium,  $\mu = 0$  and  $s = (\varepsilon + P)/T$  follows immediately. Defining the fugacity factor as  $\gamma_q = e^{\mu/T}$ , Maxwell relations give

$$n_q = \left( \frac{\partial N}{\partial V} \right)_{\mu,T} = \left( \frac{\partial P}{\partial \mu} \right)_{V,T} = \left( \frac{\partial P}{\partial \gamma_q} \right)_{V,T} \left( \frac{\partial \gamma_q}{\partial \mu} \right)_{V,T} = \frac{\gamma_q}{T} \left( \frac{\partial P}{\partial \gamma_q} \right)_{V,T}, \quad (13)$$

and thus

$$s = \frac{\varepsilon + P - \mu n_q}{T} = \frac{\varepsilon + P}{T} - \frac{\gamma_q \ln \gamma_q}{T} \left( \frac{\partial P}{\partial \gamma_q} \right)_{V,T}. \quad (14)$$

Using Eq. 4:

$$\begin{aligned} \left( \frac{\partial P}{\partial \gamma_q} \right)_{V,T} &= \left( \frac{T_c}{T_3} \right)^4 P_3 \left( T \frac{T_3}{T_c} \right) - \left( \frac{T_c}{T_0} \right)^4 P_0 \left( T \frac{T_0}{T_c} \right) \\ &\quad + \gamma_q \left( \frac{4T_c^3}{T_3^4} \right) \left( \frac{\partial T_c}{\partial \gamma_q} \right) P_3 \left( T \frac{T_3}{T_c} \right) + (1 - \gamma_q) \left( \frac{4T_c^3}{T_0^4} \right) \left( \frac{\partial T_c}{\partial \gamma_q} \right) P_0 \left( T \frac{T_0}{T_c} \right) \\ &\quad + \gamma_q \left( \frac{T_c}{T_3} \right)^4 P'_3 \left( T \frac{T_3}{T_c} \right) \left( - \frac{TT_3}{T_c^2} \right) \left( \frac{\partial T_c}{\partial \gamma_q} \right) \\ &\quad + (1 - \gamma_q) \left( \frac{T_c}{T_0} \right)^4 P'_0 \left( T \frac{T_0}{T_c} \right) \left( - \frac{TT_0}{T_c^2} \right) \left( \frac{\partial T_c}{\partial \gamma_q} \right). \end{aligned} \quad (15)$$

Using that

$$\frac{\partial T_c(\gamma_q)}{\partial \gamma_q} = \frac{1}{2\sqrt{\gamma_q}} (T_3 - T_0), \quad (16)$$

Eq. 15 becomes

$$\begin{aligned} \left( \frac{\partial P}{\partial \gamma_q} \right)_{V,T} &= \left( \frac{T_c}{T_3} \right)^4 P_3 \left( T \frac{T_3}{T_c} \right) - \left( \frac{T_c}{T_0} \right)^4 P_0 \left( T \frac{T_0}{T_c} \right) \\ &\quad + 2\sqrt{\gamma_q} (T_3 - T_0) \left( \frac{T_c^3}{T_3^4} \right) P_3 \left( T \frac{T_3}{T_c} \right) + \frac{2(1 - \gamma_q)}{\sqrt{\gamma_q}} (T_3 - T_0) \left( \frac{T_c^3}{T_0^4} \right) P_0 \left( T \frac{T_0}{T_c} \right) \\ &\quad - \frac{\sqrt{\gamma_q}}{2} \frac{T(T_3 - T_0)}{T_c} \left( \frac{T_c}{T_3} \right)^3 P'_3 \left( T \frac{T_3}{T_c} \right) - \frac{(1 - \gamma_q)}{2\sqrt{\gamma_q}} \frac{T(T_3 - T_0)}{T_c} \left( \frac{T_c}{T_0} \right)^3 P'_0 \left( T \frac{T_0}{T_c} \right). \end{aligned} \quad (17)$$

Inserting this result into Eq. 14 yields

$$\begin{aligned}
s(T, \gamma_q) = & \frac{\varepsilon(T, \gamma_q) + P(T, \gamma_q)}{T} \\
& - \frac{\gamma_q \ln \gamma_q}{T} \left( \left( \frac{T_c(\gamma_q)}{T_3} \right)^4 P_3 \left( T \frac{T_3}{T_c(\gamma_q)} \right) - \left( \frac{T_c(\gamma_q)}{T_0} \right)^4 P_0 \left( T \frac{T_0}{T_c(\gamma_q)} \right) \right) \\
& - \frac{2\sqrt{\gamma_q} \ln \gamma_q}{T} \frac{T_3 - T_0}{T_c(\gamma_q)} \left( \gamma_q \left( \frac{T_c(\gamma_q)}{T_3} \right)^4 P_3 \left( T \frac{T_3}{T_c(\gamma_q)} \right) \right. \\
& \quad \left. + (1 - \gamma_q) \left( \frac{T_c(\gamma_q)}{T_0} \right)^4 P_0 \left( T \frac{T_0}{T_c(\gamma_q)} \right) \right) \\
& + \frac{\sqrt{\gamma_q} \ln \gamma_q}{2} \frac{T_3 - T_0}{T_c(\gamma_q)} \left( \gamma_q \left( \frac{T_c(\gamma_q)}{T_3} \right)^3 P'_3 \left( T \frac{T_3}{T_c(\gamma_q)} \right) \right. \\
& \quad \left. + (1 - \gamma_q) P'_0 \left( T \frac{T_0}{T_c(\gamma_q)} \right) \left( \frac{T_c(\gamma_q)}{T_0} \right)^3 \right).
\end{aligned} \tag{18}$$

This result can be computed using the previously defined functions  $\varepsilon(T, \gamma_q)$ ,  $P(T, \gamma_q)$ , and  $T_c(\gamma_q)$ , together with the original lattice-derived pressures. This analytic expression is used to calculate the entropy in the equation of state, though it can also be shown that a similar result is found through the more straightforward numerical evaluation of

$$s(T, \gamma_q) = \frac{dP(T, \gamma_q)}{dT} = \frac{dP(T, \exp(\frac{\mu}{T}))}{dT}. \tag{19}$$

### 1.3 Speed of Sound

The speed of sound is computed through straightforward numerical differentiation:

$$c_s^2(T, \gamma_q) = \frac{dP}{d\varepsilon}(T, \gamma_q) \tag{20}$$

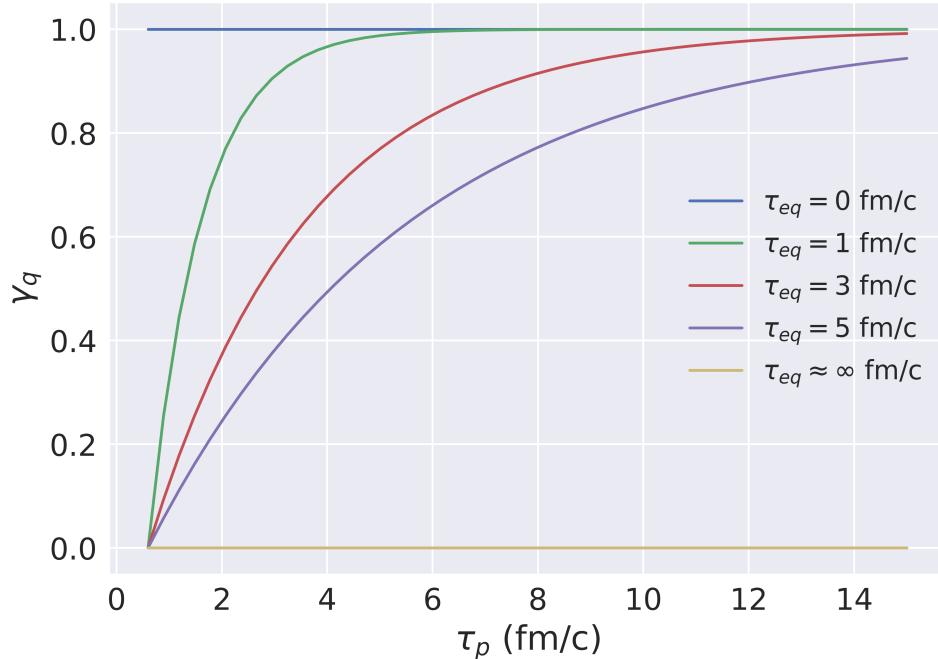
Although  $c_s^2$  does not strictly need to be tabulated, as MUSIC and similar codes can calculate the derivatives themselves, we found that the code was more stable with an externally tabulated speed of sound. Another important consideration is that in the vicinity of a phase transition, the numerically estimated  $c_s^2$  can drop to negative values, and so a minimum value of  $10^{-15}$  is enforced.

## 2 Quark Fugacity

The quark fugacity  $\gamma_q$  is parameterized as a simple function of the local proper time  $\tau_P$ :

$$\gamma_q(\tau_P) = 1 - \exp \left( \frac{\tau_0 - \tau_P}{\tau_{eq}} \right), \tag{21}$$

where  $\tau_0$  is the global initial time and  $\tau_{eq}$  is a free parameter corresponding to the effective chemical equilibration time. Figure 2 shows the form of this function.



**Figure 2:**  $\gamma_q$  as a function of proper time for several equilibration timescales  $\tau_{eq}$ .

Transverse flow will cause the local proper time of fluid cells to evolve at different rates, so during a simulation we must solve the equation

$$u^\mu \partial_\mu \tau_P = 1 \quad (22)$$

with the initial condition  $\tau_P = \tau_0$  to correctly determine the fugacity, and thus EoS, everywhere in the fluid. The result of this is that regions of the fluid with greater flow velocities will equilibrate more slowly, which typically corresponds to the periphery of the system.

### 3 Viscosity

I have used the above implementation in viscous hydrodynamics, but have not really studied yet the effects of quark chemical equilibration on the viscosities. Section 3.1 describes how we treat viscous corrections during particlization. Sections 3.2 and 3.3 describe possible ways to parameterize the shear and bulk viscosity.

#### 3.1 Viscous Corrections

At particlization, the hadron distribution functions are sensitive to both viscosities and any non-zero chemical potential. During particlization, we treat the hadron distribution functions suppressed by fugacities defined in Eq. 8 as though they were equilibrium distribution functions. We calculate the viscous corrections to the distribution functions using the 14-moment approximation, with no further modifications beyond the aforementioned change. There is no other explicit chemical potential dependence of the viscous corrections because quark number is explicitly not conserved, and so there is no conserved charge one can use to define a current as in the case of baryon chemical potential. This has been done in the particlization code iS3D [5].

### 3.2 Shear Viscosity

During hydrodynamics, the shear and bulk viscosities are not treated any differently, except that their values may change with  $\gamma_q$ . Our aim here is to be as agnostic as possible about what effect varying  $\gamma_q$  actually has. This approach may need to be modified if we end up with an excessively large parameter space. One conventional parameterization for  $\eta/s$  as a function of  $T$  in the equilibrium case is:

$$(\eta/s)_3 = \begin{cases} (\eta/s)_0 + a_h(T - T_3), & \text{if } T > T_3 \\ (\eta/s)_0 + a_l(T_3 - T), & \text{if } T < T_3 \end{cases} \quad (23)$$

where the free parameters are:

- $(\eta/s)_0$ : the minimum value at the kink.
- $a_l$ : the slope at low temperature.
- $a_h$ : the slope at high temperature.

The temperature of the minimum can also be a free parameter, but here I fix it at  $T_c$ . At arbitrary  $\gamma_q$ , here we consider the parameterization

$$(\eta/s)(T, \gamma_q) = \begin{cases} (1 - \alpha_h \gamma_q^{\beta_\eta})(\eta/s)_3(T(T_3/T_c(\gamma_q))), & \text{if } T > T_c(\gamma_q) \\ (1 - \alpha_l \gamma_q^{\beta_\eta})(\eta/s)_3(T(T_3/T_c(\gamma_q))) - (\eta/s)_0(\alpha_h - \alpha_l), & \text{if } T < T_c(\gamma_q). \end{cases} \quad (24)$$

The additional free parameters introduced here are:

- $\alpha_l$ : a coefficient for the dependence of the low temperature  $\eta/s$  on  $\gamma_q$  (independent if  $\alpha_l = 0$ ).
- $\alpha_h$ : a coefficient for the dependence of the high temperature  $\eta/s$  on  $\gamma_q$  (independent if  $\alpha_h = 0$ ).
- $\beta_\eta$ : the power dependence of  $\eta/s$  on  $\gamma_q$ .

### 3.3 Bulk Viscosity

In equilibrium,  $\zeta/s$  can be modeled as a skewed Cauchy distribution:

$$(\zeta/s)_3 = \frac{\zeta_{max} \Lambda^2}{\Lambda^2 + (T - T_3)^2} \quad (25)$$

$$\Lambda = w_\zeta [1 + \lambda_\zeta \text{sign}(T - T_3)] \quad (26)$$

where the free parameters are:

- $\zeta_{max}$ : the maximum value of the viscosity.
- $w_\zeta$ : the width of the distribution.

- $\lambda_\zeta$ : the skewness of the distribution.

We generalize to arbitrary  $\gamma_q$  by allowing these three parameters to vary as:

$$\zeta_{max}^* = \zeta_{max}(1 - \alpha_{max}\gamma_q^{\beta_\zeta}) \quad (27)$$

$$w_\zeta^* = w_\zeta(1 - \alpha_w\gamma_q^{\beta_\zeta}) \quad (28)$$

$$\lambda_\zeta^* = \lambda_\zeta(1 - \alpha_\lambda\gamma_q^{\beta_\zeta}) \quad (29)$$

to give us a complete expression

$$(\zeta/s)(T, \gamma_q) = \frac{\zeta_{max}^*(\Lambda^*)^2}{(\Lambda^*)^2 + (T - T_c(\gamma_q))^2} \quad (30)$$

$$\Lambda^* = w_\zeta^*[1 + \lambda_\zeta^*\text{sign}(T - T_c(\gamma_q))]. \quad (31)$$

The new parameters in this case are:

- $\alpha_{max}$ : a coefficient for the dependence of the maximum viscosity on  $\gamma_q$  (independent if  $\alpha_{max} = 0$ ).
- $\alpha_w$ : a coefficient for the dependence of the width on  $\gamma_q$  (independent if  $\alpha_w = 0$ ).
- $\alpha_\lambda$ : a coefficient for the dependence of the skewness on  $\gamma_q$  (independent if  $\alpha_\lambda = 0$ ).
- $\beta_\zeta$ : the power dependence of  $\zeta/s$  on  $\gamma_q$ .

## 4 Strangeness

When separating light and strange quarks, our plan is to use the same time-dependent fugacity function in Eq. 21, only separated into two copies:

$$\gamma_l(\tau_P) = 1 - \exp\left(\frac{\tau_0 - \tau_P}{\tau_{l,eq}}\right) \quad (32)$$

$$\gamma_s(\tau_P) = 1 - \exp\left(\frac{\tau_0 - \tau_P}{\tau_{s,eq}}\right), \quad (33)$$

where  $\gamma_l$  and  $\gamma_s$  are the light and strange fugacities, respectively, and  $\tau_{l,eq}$  and  $\tau_{s,eq}$  are independent free parameters defining their equilibration times.

For the equation of state itself, it would be simplest to maintain exactly the same construction and define the total quark fugacity as

$$\gamma_q = \frac{2}{3}\gamma_l + \frac{1}{3}\gamma_s, \quad (34)$$

as it would require even bolder assumptions than we have already made to define an explicitly flavor-dependent equation of state where some quark flavors are suppressed more than others.

In principle, one can define the hadron fugacities in terms of quark fugacities as something like [6]:

$$\lambda_i = \gamma_u^{N_u^i} \gamma_d^{N_d^i} \gamma_s^{N_s^i} \gamma_{\bar{u}}^{N_{\bar{u}}^i} \gamma_{\bar{d}}^{N_{\bar{d}}^i} \gamma_{\bar{s}}^{N_{\bar{s}}^i}. \quad (35)$$

We have thus far simplified this to a single factor with a power of 2 for mesons and 3 for baryons by treating quark flavors symmetrically. When differentiating light and strange quarks, assuming we maintain zero baryon chemical potential, we would have to calculate truly species-specific fugacities of the form

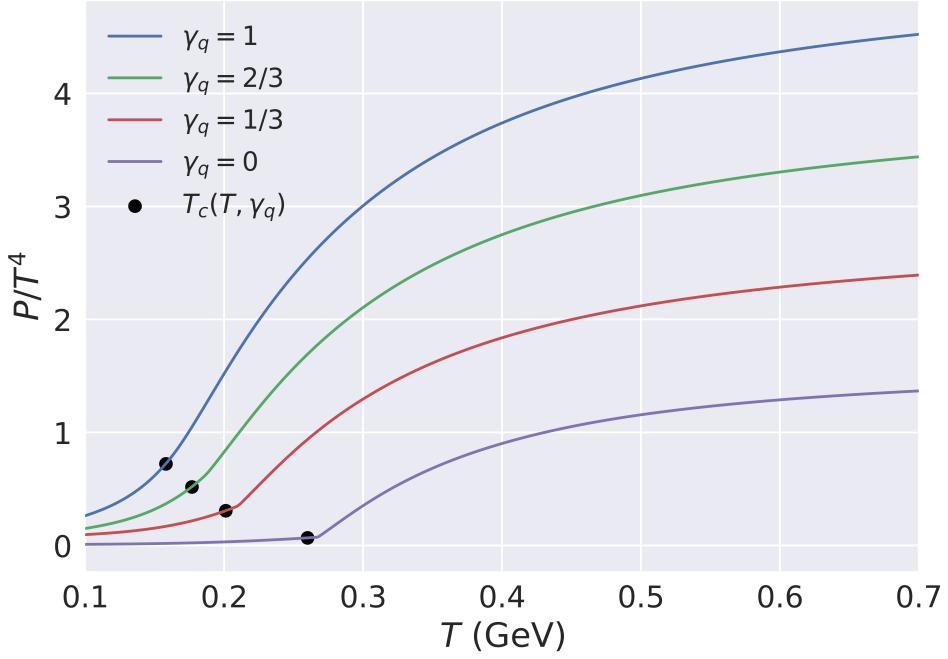
$$\lambda_i = \gamma_l^{N_l^i} \gamma_s^{N_s^i}, \quad (36)$$

and use them to replace all of the  $\lambda_i$  above.

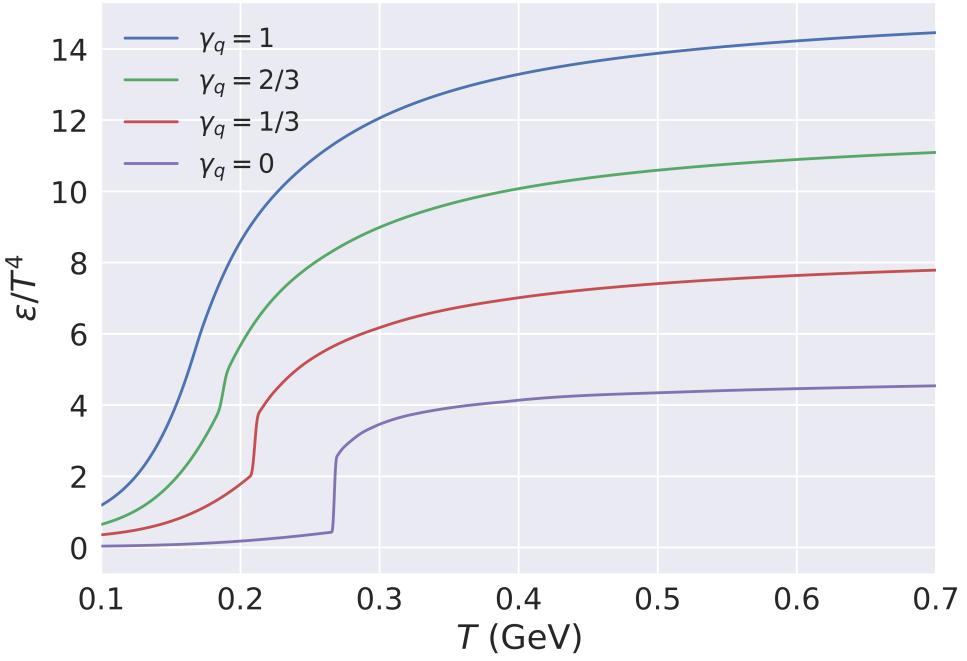
## 5 Results

$\varepsilon, P, s, T$ , and  $c_s^2$  are computed according to the steps in Section 1 and tabulated with even spacing in  $\varepsilon^{1/4}$  (the power is for numerical interpolation reasons) and  $\gamma_q$ . This is the file which is read by MUSIC, which calculates  $\gamma_q(\tau_p)$  and then simply performs a 2D interpolation across  $\varepsilon$  and  $\gamma_q$  to find  $P, s, T$ , and/or  $c_s^2$  for any given fluid cell.

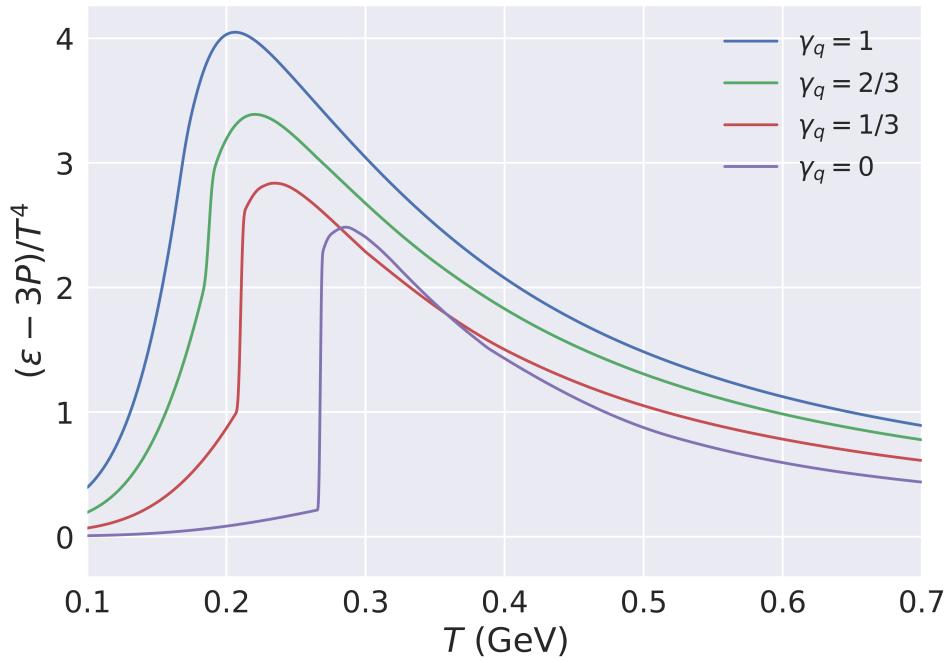
The following figures show all of the tabulated quantities for the PCE equation of state.



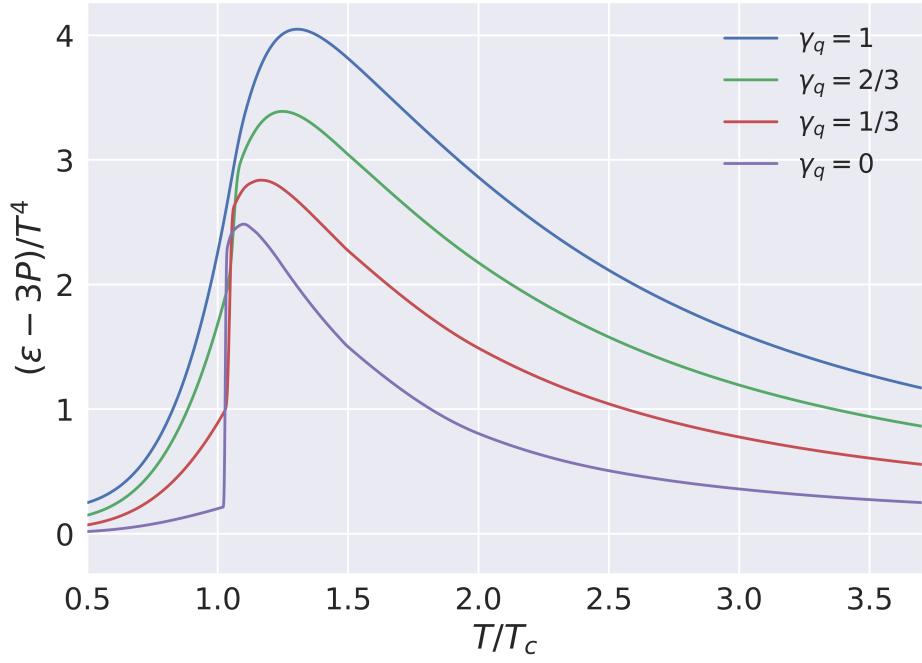
**Figure 3:** Interpolated  $P/T^4$  as a function of temperature for several choices of  $\gamma_q$ . The black points show the location of the critical temperature for each  $\gamma_q$ .



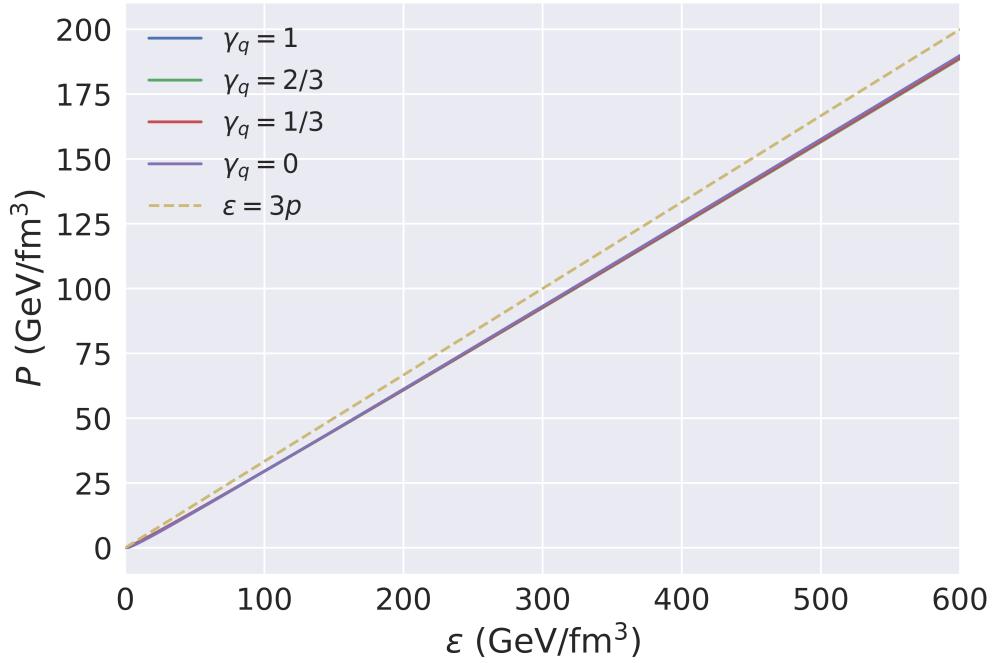
**Figure 4:** Interpolated  $\varepsilon/T^4$  as a function of temperature for several choices of  $\gamma_q$ .



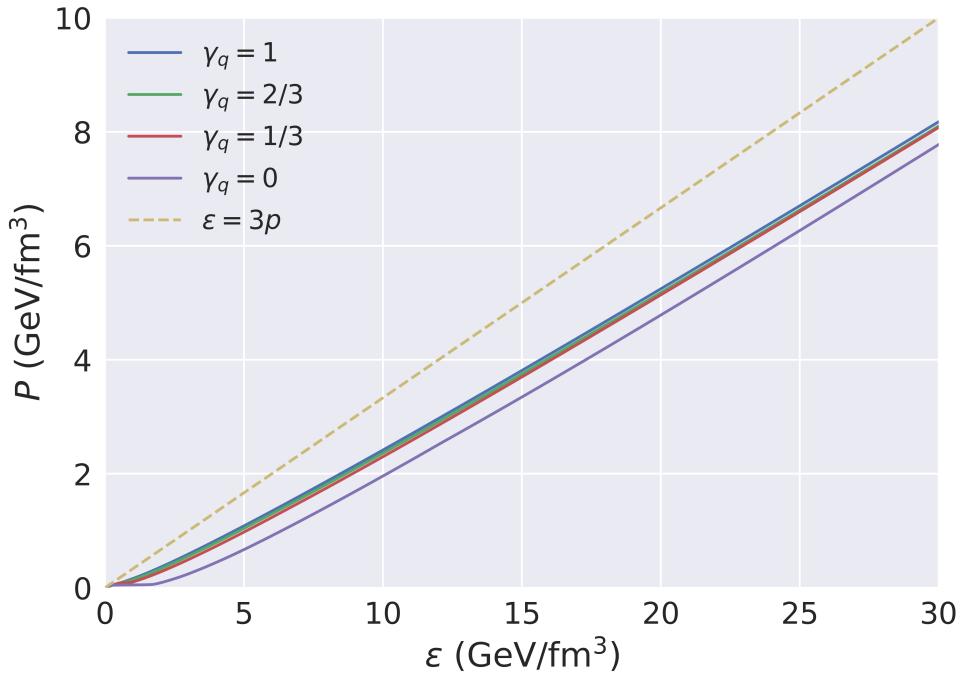
**Figure 5:** Trace anomaly  $\Theta^{\mu\mu}/T^4 = (\varepsilon - 3P)/T^4$  for several choices of  $\gamma_q$ .



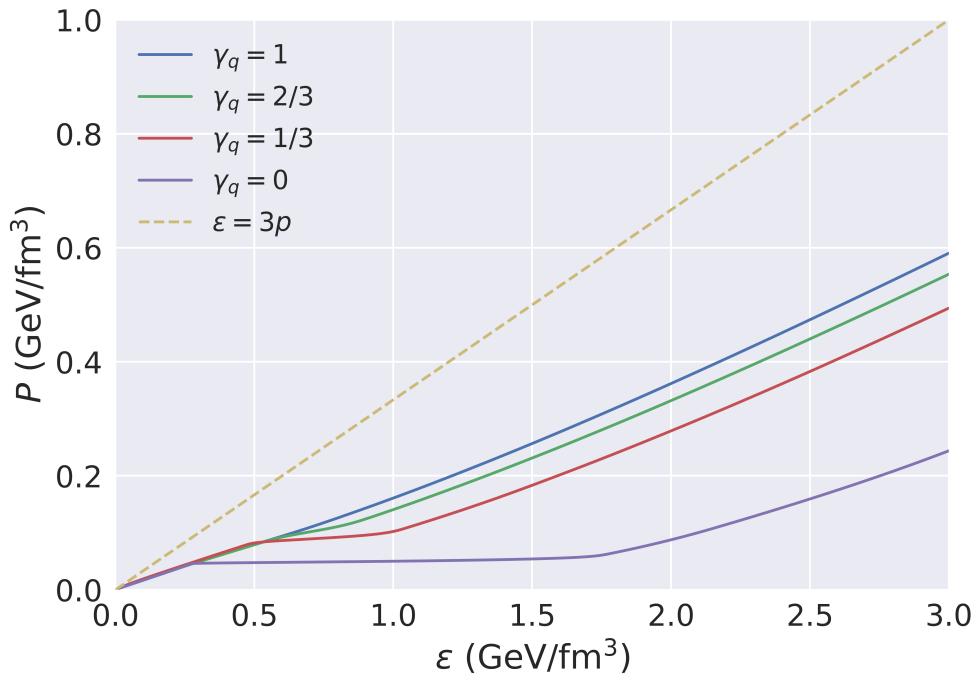
**Figure 6:** Trace anomaly as above, but plotted against  $T/T_c(T, \gamma_q)$ .



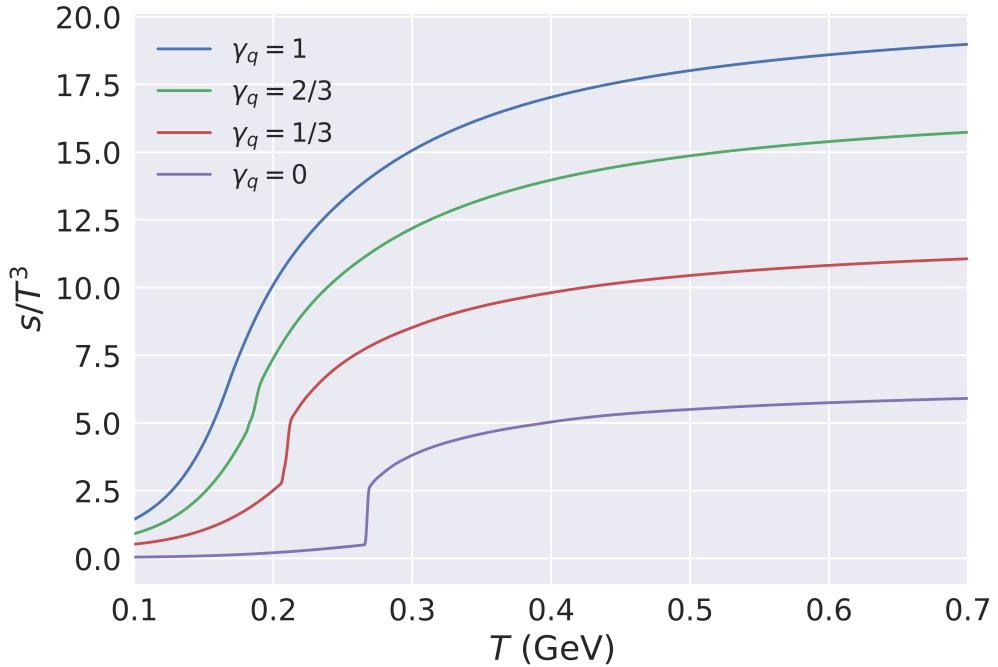
**Figure 7:** Pressure as a function of energy density for several choices of  $\gamma_q$ , compared to the conformal equation of state.



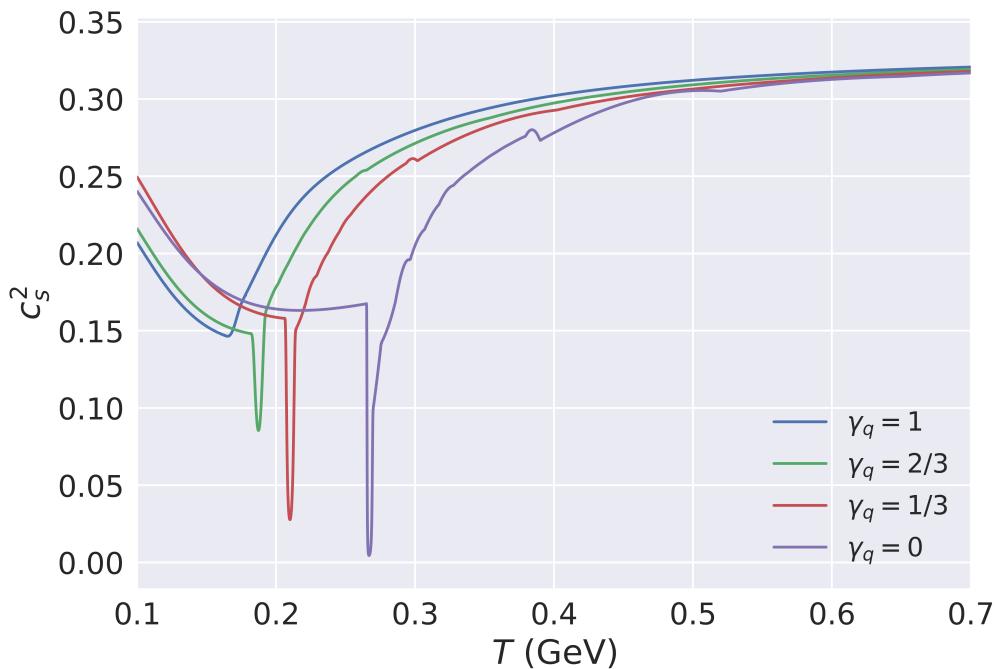
**Figure 8:** Pressure as a function of energy density as above, only zoomed in to better differentiate the curves.



**Figure 9:** Pressure as a function of energy density as above, only zoomed in further to show the behavior at the phase transition



**Figure 10:** Calculated  $s/T^3$  as a function of temperature for several choices of  $\gamma_q$ .



**Figure 11:** Calculated  $c_s^2$  as a function of temperature for several choices of  $\gamma_q$ .

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