Computational Attempt to Implement the Full Boltzmann Collision Operator

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Abstract

Thermal interaction of particles is one of the most information rich aspects of particle physics and cosmology. We can find out a lot about the nature of early universe physics by turning to what types of interactions produce measurable and detectable effects in our universe today. Scholars use the Cosmic Microwave Background (CMB) and large scale structure (LSS) analysis to create and rule out different dark matter models. The CMB and LSS provide insight into how dark matter interacts with regular matter (or baryons). In research done so far, (cold) dark matter has been assumed to interact efficiently with itself, so as to have a Maxwell-Boltzmann distribution. However, that might not be the case, and in that scenario, the full Boltzmann collision operator needs to be evaluated. Implementing the full Boltzmann operator is a very complicated task, and in this project, I have tried to create the initial structure of the code using a simple case. My code will take a temperature profile, $T(t)$, and a differential scattering rate, (Γ), to find the how the distribution would behave. The motivation of this project was to find a way to implement the full Boltzmann Collision Operator (for some specific simplified cases) and compare how much better the Fokker-Planck approximation is compared to the efficient self-interacting dark matter (or the Maxwell-Boltzmann) assumption.

1 Introduction

The nature of thermal interactions between dark matter particles and regular matter (baryons) leaves detectable information on observables such as the Cosmic Microwave Background (CMB) or on large scale structure of the universe. The way the observable effects are predicted depends on the model of dark matter, dark matter-baryon interaction cross-section, and dark matter self-interactions. In the literature that exists so far, dark matter self-interactions are assumed to be efficient such that the dark matter distribution behaves as Maxwell-Boltzmann. However, this might not be the correct assumption to make because dark matter might interact weakly with itself. In this case, the evolution of the distribution function f_χ is governed by the full Boltzmann collision operator, $C[f_\chi]$. In [1], there is detailed analysis of dark matter (DM) self-interactions which are not assumed to be efficient enough to behave as Maxwell-Boltzmann. A Fokker-Planck approximation to the Boltzmann collision operator is found in [1]. This paper is one of my main sources for this

project as it provides the context and motivation for why we might need implementation of the full Boltzmann collision operator.

In general, any implementation of the Boltzmann collision operator should (1) obey detailed balance, (2) conserve the total number of particles in the distribution, and (3) satisfy the theoretical heating and momentum exchange rates. It is important to work towards finding a computational scheme which satisfies the three conditions mentioned above and that is the goal of this ongoing project. The code for the completed parts of this project is fairly straightforward: I use the Runge-Kutta method for time evolution and a centered difference scheme for spatial derivatives.

The rest of this report is organized as follows: In §2 I give an introduction to concepts which are central to the physics behind this project, in §3 I discuss the computational methods which have been implemented, §4 records my attained results. I conclude in §5 with a discussion of where the results fit into the problem in general, and the parts which I could not complete and are future work.

2 The Physics of the Problem

2.1 Scattering Theory

The problem we are interested in is simplified to consider elastic collisions between point-like DM particles (represented by the subscript χ throughout the report) and any other baryonic scatterer, s (protons, electrons, etc). The initial velocities are $\boldsymbol{v_\chi}$ and $\boldsymbol{v_s}$ which scatter into $\boldsymbol{v'_\chi}$ and $\boldsymbol{v'_s}$ such that energy and momentum are conserved in a $\chi + s \to \chi + s$ interaction. By conservation of energy and momentum, we can conclude that $|\boldsymbol{v_\chi} - \boldsymbol{v_s}| = |\boldsymbol{v'_\chi} - \boldsymbol{v'_s}|$. To define other notation, $\boldsymbol{v_\chi} - \boldsymbol{v_s} \equiv \boldsymbol{v_{\chi s}}$ and $\boldsymbol{v'_\chi} - \boldsymbol{v'_s} \equiv \boldsymbol{v'_{\chi s}}$. The unit vectors $\hat{n}$ and $\hat{n}'$ correspond to the directions of the initial and final velocities $\boldsymbol{v_{\chi s}}$ respectively (notation same as in [1]).

Two significant concepts in scattering theory are cross-section, σ, and differential cross-sections of an interaction, $\frac{d\sigma}{d\Omega}$. The cross-section of a collision determines how probable it is for two particles to collide. It is directly related to the face-on area of a the target. The cross-section that appears in [1], and the one that governs the theory of this project is the momentum transfer cross-section which depends on the velocity difference $v_{\chi s}$,

$$\sigma(v_{\chi s}) = \int d^2\hat{n}' \frac{d\sigma_{\chi s}}{d\Omega}(1 - \hat{n} \cdot \hat{n}') \tag{1}$$

Differential cross-section $\frac{d\sigma}{d\Omega}$ (which also appears in eq. 1) is the ratio between the infinitesimal cross-section $d\sigma$ that a particle sees and the infinitesimal solid angle $d\Omega$ which it scatters into [2]. It should be noted that the total cross-section is obtained by integrating over all possible scattering solid angles.

2.2 Boltzmann Collision Operator

The Boltzmann collision operator $C[f](v)$ is a measure of how the distribution of velocities ($f(\boldsymbol{v_\chi})$ in this particular case) changes over time for a collisions

between two specific populations of particles. So essentially [1],

$$C[f_\chi] = \frac{df_\chi}{dt} \tag{2}$$

More formally, the collision operator $C_{\chi s}[f_\chi](\boldsymbol{v_\chi})$ depends on the differential scattering rate, Γ, which is the operator which determines how two populations of particles exchange velocities. $f(\boldsymbol{v'_\chi})\Gamma(\boldsymbol{v'_\chi} \to \boldsymbol{v_\chi})$ is the quantity which tells us the rate at which particles in f_χ which have initial velocity $\boldsymbol{v'_\chi}$ scatter into the final velocity $\boldsymbol{v_\chi}$. Thus, we understand $\Gamma(\boldsymbol{v'_\chi} \to \boldsymbol{v_\chi})$ as the rate at which velocities are coming "in" to $\boldsymbol{v_\chi}$ and $\Gamma(\boldsymbol{v_\chi} \to \boldsymbol{v'_\chi})$ as the rate of velocities going "out" of $\boldsymbol{v_\chi}$. We would intuitively anticipate, that the evolution of $f(\boldsymbol{v_\chi})$ would depend on the difference of particles entering into $\boldsymbol{v_\chi}$ and those leaving $\boldsymbol{v_\chi}$ in velocity phase space. Then, we have [1],

$$C_{\chi s}[f_\chi](\boldsymbol{v_\chi}) = \int d^3v'_\chi \left\{ f_\chi(\boldsymbol{v'_\chi})\Gamma_{\chi s}(\boldsymbol{v'_\chi} \to \boldsymbol{v_\chi}) - f_\chi(\boldsymbol{v_\chi})\Gamma_{\chi s}(\boldsymbol{v_\chi} \to \boldsymbol{v'_\chi}) \right\} \tag{3}$$

Γ itself is obtained from the differential momentum cross-section, and the scatterer population, $f_s(\boldsymbol{v_s})$,

$$\begin{aligned} \Gamma_{\chi s}(\boldsymbol{v_\chi} \to \boldsymbol{v'_\chi}) \equiv n_s \int d^3v'_s f_s(\boldsymbol{v_s}) v_{\chi s} \int d^2\hat{n}' \frac{d\sigma_{\chi s}}{d\Omega} \\ \delta_D \left(\boldsymbol{v'_\chi} - \boldsymbol{v_\chi} - \frac{m_s}{(m_\chi + m_s)} v_{\chi s}(\hat{n}' - \hat{n}) \right) \end{aligned} \tag{4}$$

where m_χ and m_s refer to mass of particles in the respective populations, and the Dirac delta function imposes conservation of energy and momentum.

It should be noted that as mentioned before, $\Gamma_{\chi s}$ should obey detailed balance. Detailed balance is a property which ensures that if a population is in thermal equilibrium, it should remain so. That is, if $f(\boldsymbol{v_\chi})$ is Maxwell-Boltzmann (essentially, a Gaussian distribution), then the scattering rates should be such that $\frac{df_\chi}{dt} = 0$. Therefore, explicitly, in thermal equilibrium, $f(\boldsymbol{v_\chi})$ should take the form [1]

$$f_{eq}(\boldsymbol{v_\chi}) = \left(\frac{m_\chi}{2\pi T_\chi} \right)^{3/2} \exp\left(-\frac{m\boldsymbol{v_\chi}^2}{2T_\chi} \right) \tag{5}$$

Moreover, we should also ensure that any modeling of $C_{\chi s}[f_\chi](\boldsymbol{v_\chi})$ should not change the number of particles in the distribution. As it can be seen, and will be explicitly verified later, eq. 3 conserves particle number.

3 Computational Methods

3.1 Setting up the Problem

Our main goal is to computationally implement eq. 3. Since we are considering an isotropic universe, our problem becomes dependent essentially on just the magnitudes of velocities, and not their direction. Motivated by the form of the exponential in eq. 5, we define a dimensionless velocity,

$$u \equiv \sqrt{\frac{m}{T(t)}} v \tag{6}$$

In terms of the dimensionless velocity, the form of $C[f_\chi](v_\chi)$ changes as $\frac{df_\chi(v_\chi)}{dt} \to \frac{df_\chi(u)}{dt}$, where by the chain rule of differenciation,

$$\frac{df_\chi(u)}{dt} = \frac{\partial f_\chi}{\partial t} + \frac{du}{dt}\frac{\partial f_\chi}{\partial u}$$

Our main objective is to solve for

$$\frac{\partial f_\chi}{\partial t} = \frac{df_\chi(u)}{dt} - \frac{du}{dt}\frac{\partial f_\chi}{\partial u} \tag{7}$$

The first term in eq. (7) is found by discretizing eq. (3) and making it into a single integral by adding a prefactor (because of dependence only on magnitudes of velocities, we do not need a 3D integral). The discretized form of eq. (3) is as follows:

$$\left(\frac{df}{dt}\right)_i = 4\pi u_j^2 \Delta u \sum_j \left(\Gamma_{ji} f_j - f_i \Gamma_{ij}\right), \tag{8}$$

where Γ_{ij} is the matrix element of a chosen Γ which satisfies detailed balance,

$$\Gamma_{ij} \equiv \left(\frac{1}{2\pi}\right)^{3/2} \exp\left(-\frac{1}{2}u_j^2\right) \tag{9}$$

It can be checked that this choice of Γ satisfies detailed balance,

$$\exp\left(-\frac{1}{2}u_i^2\right)\Gamma_{ij} = \exp\left(-\frac{1}{2}u_j^2\right)\Gamma_{ji} \tag{10}$$

Ideally, Γ should not have been curated to obey detailed balance, but derived from the cross-section $\sigma_{\chi s}$. However, that requires implementing eq. (4), which is not a trivial task. This is the case because the 3D Dirac delta function in the second integral has $v_{\chi s}$ within it which is dependent on $f_s(\boldsymbol{v_s})$ in the first integral. A lot of time that I worked on this project towards the end was spent on trying to simplify eq. (4), but I was not able to succeed. I will discuss my attempts briefly in the concluding section.

The second term in eq. (7) has a coefficient which can be determined using eq. (6),

$$\frac{du}{dt} = -\frac{1}{2}u\frac{d\ln T}{dt}$$

Then, $\frac{\partial f}{\partial u}$ is found using a centered difference scheme.

Before diving into implementing eq. (7), we do one more change of variables, so that the distribution function has a modified form which is actually analogous to the number of particles normalized to 1. We define

$$N \equiv \left(\frac{T(t)}{m_\chi}\right)^{3/2} u^2 f_\chi(u) \tag{11}$$

An additional advantage of this change of variables is that the boundary conditions become trivially 0 at both ends of the distribution. So now we would alternatively like to find

$$\left(\frac{\partial N}{\partial u}\right)_i = \frac{3}{2}\frac{d\ln T}{dt}N_i + u_i^2\left(\frac{T}{m}\right)^{3/2}\left(\frac{\partial f}{\partial t}\right)_i \tag{12}$$

To find $\left(\frac{\partial f}{\partial t}\right)_i$ in terms of N, in eq. (8), we simply replace

$$f_i = \left(\frac{m_\chi}{T}\right)^{3/2} \frac{N_i}{u_i^2},$$

and in eq. (7) we replace

$$\frac{\partial f_\chi}{\partial u} = \left(\frac{m_\chi}{T}\right)^{3/2} \left(\frac{1}{u_i^2}\frac{\partial N_i}{\partial u} - \frac{2N_i}{u_i^3}\right).$$

Finally, the equation which we implement using Runge-Kutta and centered difference is

$$\frac{\partial N_i}{\partial t} = \left(\frac{T(t)}{m}\right)^{3/2} 4\pi\ \Delta u \sum_j \left(\Gamma_{ji} N_j u_i^2 - N_i u_j^2 \Gamma_{ij}\right) + \frac{1}{2}\frac{d\ln T}{dt}\left(u_i \frac{\partial N_i}{\partial u} + N_i\right) \tag{13}$$

As a sanity check, we must ensure that $\frac{\partial N_i}{\partial t} = 0$, because the normalized number of particles should always remain unchanging. It can analytically be checked that all terms in eq. (13) add up to 0.

3.2 Time Evolution

This project clearly demands a time-evolution code, and for that I used the fourth order Runge-Kutta method (RK-4). A Runge Kutta method solves for any ordinary differential equation of the form

$$\frac{df(t)}{dt} = f'(t) = g(f(t), t)$$

if we have the function $g(f(t), t)$ and $f(t = 0) = f_0$ [3]. In the case of this project, $g(f(t), t)$ takes the form of eq. 3. The RK-4 method is a higher-order method with accuracy up to $\mathcal{O}(\epsilon^5)$. The algorithm calculates $\Delta f(t)$ over a time step (say, $t \to t + h$), in four distinct steps, as follows:

1. Starting from an initial function $f_0(v, t_0)$, we find the derivative at t_0, f_1', such that $f_1' * h$ can be thought of as a first approximation of Δf.

$$f_1' = g(f_0, t_0)$$

2. However, since $\Delta f = f_1' * h$ would only be first order accurate, we use it to find the value of $f(v, t)$ at $t = t_0 + \frac{h}{2}$, and use that value of f to find the slope at $t_0 + h$.

$$f_2' = g(f_0 + f_1' * \frac{h}{2}, t_0 + \frac{h}{2})$$

3. The value of the slope which f_2' provides is then used to again find the value of the function at $t_0 + \frac{h}{2}$. Then that estimate of f is used to find the slope at the half time-step.

$$f_3' = g(f_0 + f_2' * \frac{h}{2}, t_0 + \frac{h}{2})$$

4. Finally then, f_3' is used to step all the way to $t_0 + h$.

$$f_4' = g(f_0 + f_3' * h, t_0 + h)$$

Putting it all together, we find the full time-step difference using a weighted average,

$$f(v, t_0 + h) = f_0(v, t_0) + h * \left(\frac{f_1'}{6} + \frac{f_2'}{3} + \frac{f_3'}{3} + \frac{f_4'}{6} \right)$$

3.3 Centered Difference

The method to find the partial spatial derivative $\frac{\partial N_i}{\partial u}$, I used a fairly straightforward centered difference scheme. The idea behind centered difference is to approximate the derivative of a function $f'(u_i)$ at some value by a polynomial by using the information available around u_i. If the grid spacing is small enough, then we can approximate the exact derivative with the polynomial [4]. Specifically,

$$\frac{\partial N_i}{\partial u} = \frac{N_{i+1} - N_{i-1}}{2\Delta u}$$

3.4 Time-Dependent Temperature

In an expanding universe, space between all matter increases with "velocities" given by the Hubble expansion rate, H, which is defined on the basis of the dimensionless scale factor a of the universe. So it is essentially the scale factor which is a measure of how distances change in the universe over time [5].

After the Big Bang, as space between matter (and radiation) increases, their interactions become less frequent and different populations of particles emerge from the combined plasma begins as they fall out of thermal equilibrium. This process is known as *decoupling*. This project is concerned with non-relativistic DM decoupling and interacting with baryons in the radiation dominated era, when $a \propto t^{1/2}$ [1, 6]. As we would expect, decrease in interaction rates due to expansion changes the temperature of the distributions of particle species as $T \propto 1/a^2$.

4 Results

Now the context has been put in place to show my obtained results. As explained earlier, we would like to have a code which governs evolution of a distribution such that it only deviates from a Maxwell-Boltzmann distribution when not in thermal equilibrium. On the other hand, if there is thermal equilibrium, every distribution should evolve to become Maxwell-Boltzmann. This is a crucial test which tells us whether or not we are seeing correct time evolution of f_χ.

4.1 Thermal Equilibrium

In the case where the distribution is initially Maxwell-Boltzmann, and remains in thermal equilibrium with surrounding plasma, we should see absolutely no change over time. So if initally,

$$N(u) = 4\pi u^2 \left(\frac{1}{2\pi} \right)^{3/2} \exp\left(-\frac{u^2}{2} \right) \tag{14}$$

it should not change over time.

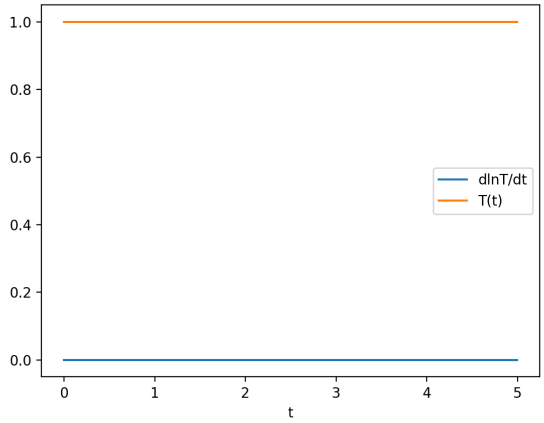

Figure 1: This figure shows the temperature profile and the rate of change of temperature imposed on the distribution $N(u)$ when the particles are in thermal equilibrium, i.e., the temperature of the bath is not changing, and the derivative is zero.

Figure 1 shows the temperature profile, which is simply constant over time, and the derivative is hence zero. The results of evolution of a Maxwell-Boltzmann (MB) distribution are also shown in figure 2. As expected, we see no change over time in the distribution.

In thermal equilibrium, we also expect that a distribution which does not start out as Maxwell-Boltzmann (but still has normalized number = 1), will approach the form of an MB distribution over time. So, with the same temperature profile as in figure 1, we find that a distribution with initial form,

$$N = \frac{1}{2\pi}\left(1 + \sin(u - \frac{\pi}{2})\right)$$

will approach eq.(14). Figure 3 shows that a non-MB distribution pretty quickly approaches MB, and then stays the same over time.

4.2 Temperature Gradient

In the case where temperature changes with time, we should expect the distributions to deviate from Maxwell-Boltzmann. Figure 4 shows an artificial temperature profile which we used to test our implementation of the code. At initial times, when the temperature is not changing very much, the distribution should be in quasi-thermal equilibrium. However, at intermediate times, when there is a large temperature gradient, the distribution should deviate from MB. Towards the end, the distribution should approach MB because the gradient is close to zero once again. Figure 5 shows precisely this type of behavior.

Moreover, we also want that a distribution which does not start out as MB displays characteristics consistent with our expectations. So, if we start with a non-MB distribution, it should approach MB whenever under a very

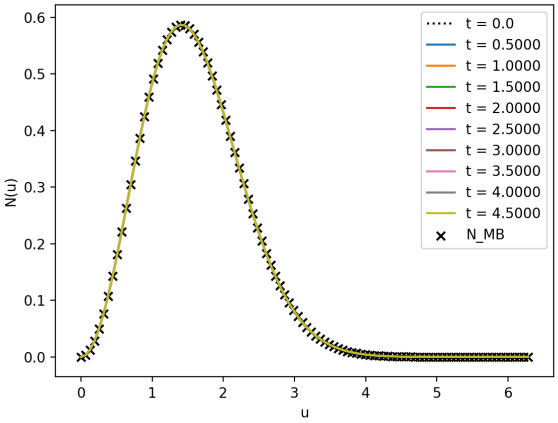

Figure 2: This figure shows how a Maxwell-Boltzmann distribution would evolve under thermal equilibrium. As we can see, that the x's marking an MB distribution coincide with the initial and each of the following time-evolved states of the population. This confirms that a distribution which already has the form of an MB Gaussian, will not evolve under thermal equilibrium.

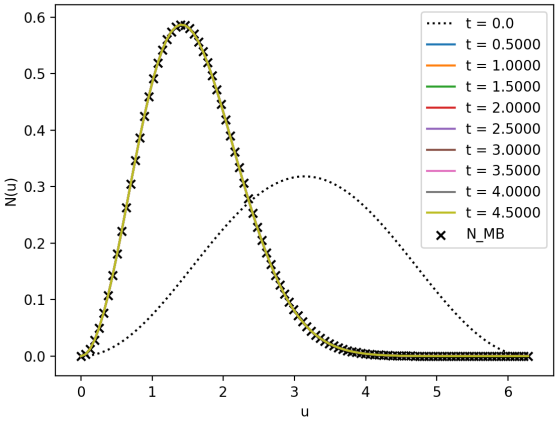

Figure 3: This figure shows how a Maxwell-Boltzmann distribution would evolve under thermal equilibrium. As we can see, the initial distribution function shown by the dotted line changes to an MB distribution coinciding with the x's, and stays the same thereafter.

slight temperature gradient. Figure 6 shows this expected behavior when a distribution evolving under the same temperature profile as figure 4.

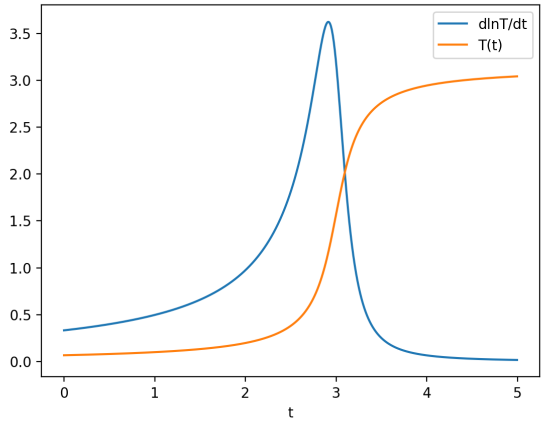

Figure 4: This figure shows an artificial temperature gradient that has been imposed on the distribution. The reason we have chosen this profile is because initially it has a slight gradient which steepens, but then flattens out again at later times. We would expect that the times when the gradient is close to zero are when the distribution would remain Maxwell-Boltzmann.

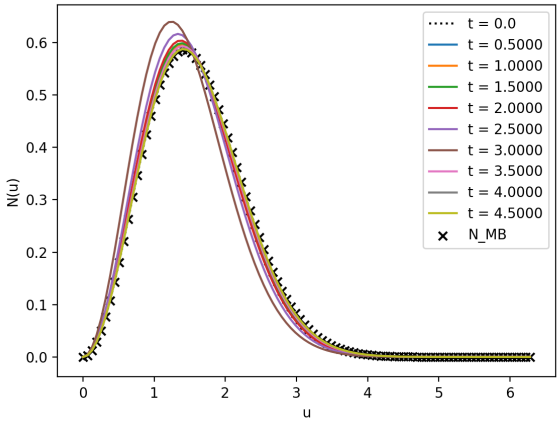

Figure 5: This figure shows how the distribution would evolve under an artificial temperature gradient. Initially, starting from an MB distribution, it can be seen that there is deviation from MB at the times of changing temperature. However, as the temperature gradient reduces and approaches zero, the distribution again returns to MB.

5 Conclusions

This project began with the motivation to be able to compare the Fokker-Planck approximation of the Boltzmann Collision Operator in a particular case to the implementation of the full operator. So far, we have been able to implement

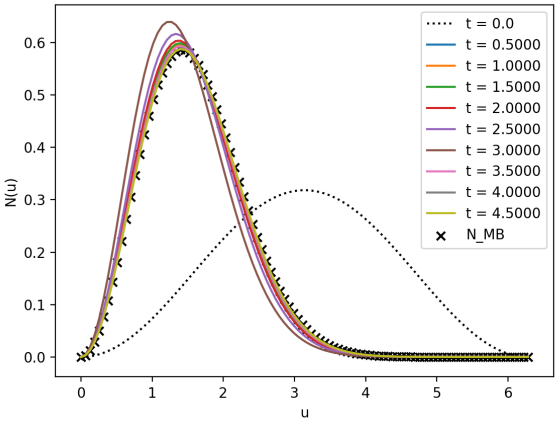

Figure 6: This figure shows how a non-MB distribution would evolve under an artificial temperature gradient. Initially, starting from an sine function distribution, it can be seen that there is deviation from MB at the times of changing temperature. However, as the temperature gradient reduces and approaches zero, the distribution approaches MB.

working code which can take a temperature profile, and a Γ matrix, and correctly evolve a particle distribution function in phase space.

Further work on this project requires that a proper temperature profile be implemented which theoretically matches the evolution in the radiation dominated era of the universe. Moreover, eq. (4) needs to be implemented computationally, or analytically to impose physically relevant time-evolution. Towards the end, I was trying to find methods to simplify the full equation for Γ. I came across computational δ function implementations which used Fourier transforms, and theoretical methods which express

$$\delta_D(f(x)) = \left|\frac{df}{dx}\right|^{-1}_{x_0} \delta_D(x - x_0)$$

where x_0 is where $f(x) = 0$. However, in the time that I had remaining, I was not able to put these methods together in a way that gave a clean form for the double integral in eq.(4). The biggest issue is to simplify the inner integral such that the dependence of $v_{\chi s}$ inside the δ function on v_s in the outer integral becomes analytically tractable.

Over the course of the past few weeks, we were able to formulate a code which has the bare bones of what needs to be done. A lot more work will go into theoretical techniques for simplifying the form of Γ, and then comparing the results to the Fokker-Planck approximation implemented in [1].

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