Lithium Diffusion in the Post-Recombination Universe and Spatial Variation of [Li/H]

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The observed amount of lithium for low metallicity population II stars (known as the Spite plateau) is a factor of \(3 - 5\) lower than the predictions of the standard cosmology. Since the observations are limited to the local Universe (halo stars, globular clusters and satellites of the Milky Way) it is possible that certain physical processes may have led to the spatial separation of lithium and local reduction of [Li/H]. We study the question of lithium diffusion after the cosmological recombination in sub-Jeans dark matter haloes, taking into account that more than 95% of lithium remains in the singly-ionized state at all times. Large scattering cross sections on the rest of the ionized gas leads to strong coupling of lithium to protons and its initial direction of diffusion coincides with that of H\(^+\). In the rest frame of the neutral gas this leads to the diffusion of H\(^+\) and Li\(^+\) out of overdensities with the trend of reducing [Li/H] in the minima of gravitational wells relative to the primordial value. We quantify this process and argue that, with certain qualifications, it may have played a significant role in creating local lithium deficiency within the primordial dark matter haloes, comparable to those observed along the Spite plateau.

The primordial abundances of light elements, \(^4\)He, D, and \(^7\)Li, offer unique window into the very early Universe at redshifts of \(z \sim 10^4\). In recent years, this probe has been sharpened: the only free parameter that enters the standard big bang nucleosynthesis (SBBN) calculations – baryon-to-photon ratio \(\eta_b\) – has been measured to great accuracy via the CMB experiments. The prediction for the primordial fraction of \(^7\)Li is \([7\text{Li}/\text{H}]_{\text{SBBN}} = (5.07^{+0.71}_{-0.67}) \times 10^{-10}\) (see e.g. \([1]\)), which is a factor of \(3 - 5\) smaller than the Spite plateau value of \([7\text{Li}]\), \((1.23^{+0.34}_{-0.16}) \times 10^{-10}\) \([2]\), an observationally determined value of the lithium abundance in the atmospheres of hot Population II halo stars. It is unclear whether stellar depletion of Li could account for such a large deficit, and speculations of non-standard physics being behind the discrepancy flourished (see, e.g. reviews \([3]\)). Most recently, this lithium problem has been further complicated by the observation of the deterioration of the plateau at the lowest metallicities, \(Z < 1.5 \times 10^{-3}\), where the discrepancy with SBBN value becomes even larger \([1]\). This might be pointing towards additional “missing” pieces of physics unrelated to the stellar physics, starting from evolution of primordial gas leading to the formation of PopII stars with lowest metallicities.

It is important to realize that the observations of lithium abundance along the Spite plateau reflect the “local” formation environments of the oldest stars in our Galaxy, while the SBBN predictions are “global”. Non-standard cosmology with an \(O(1)\) downward fluctuation of baryon-to-photon ratio in the patch of the Universe that includes Milky Way can give \([7\text{Li}/\text{H}]_{\text{local}} < [7\text{Li}/\text{H}]_{\text{SBBN}}\). However, the standard physics processes may also lead to the local under- or over-abundance of lithium relative to the SBBN prediction. In standard cosmology, the spatial fluctuations of \([7\text{Li}/\text{H}]\) are initially small, but consequently amplified by the growth of structure in combination with diffusional processes in the Early and Late Universe.

The existing astrophysical literature covers the diffusion of elements in stellar atmospheres and in the clusters of galaxies \([6,8]\). In contrast, the studies of primordial element diffusion in the early Universe are very sparse. Ref. \([9]\) addresses the evolution of elemental abundance in the linear regime, \(\delta_\rho/\rho \ll 1\). Although the linear regime by definition does not allow for large effects in the abundances, \([9]\) find that qualitative trend is such that lithium, owing to its larger mass, tends to accumulate more in the minima of gravitational potentials compared to hydrogen. Since the star formation should also occur inside gravitational wells, the qualitative trend inferred from \([9]\) is \([7\text{Li}/\text{H}]_{\text{local}} > [7\text{Li}/\text{H}]_{\text{SBBN}}\), which does not help to solve the lithium problem in any way. There is, however, an important assumption made about the neutrality of lithium in \([9]\), which does not hold in the early Universe. In fact, after the H recombination, lithium exists predominantly in the singly-ionized state, Li\(^+\) \([10]\). There are two reasons for that: firstly, the 5.39 eV ionization potential for lithium means that the recombination temperature is smaller than that of H by the factor of \(\sim 2.5\), at which time the density of the free electrons is depleted, and the recombination rates for Li are less than the Hubble expansion rate. In addition, the non-thermal population of photons from residual \(e^- - p\) recombination causes photo-ionization of neutral Li fraction and keeps its abundance below a few percent level throughout the cosmic history all the way to reionization at \(z \sim 10\) \([10]\).

In this paper, we show that the fact that lithium remains in the Li\(^+\) state has direct consequences for its diffusion after hydrogen recombination. In particular, we show that owing to the large scattering cross section on protons, Li\(^+\) stays spatially bound to H\(^+\), and the direction of their diffusion is against the gravitational force.
in the rest frame where the neutral hydrogen. From our analysis it follows that \( \frac{[Li]/H}{\text{grav} \min} < \frac{[Li]/H}{\text{SBBN}} \), which can have significant implications for the cosmological lithium problem. In the rest of the paper, we expand on this observation in some detail.

Direction of Lithium Diffusion. We consider the equations for cosmological fluids of different primordial species with number densities \( n_a \), where \( a \) spans \( H, ^{4}He, e, p, ^{7}Li \). Note that after most of the hydrogen becomes neutral, the recombination rate for residual \( e \) and \( p \) is much smaller than the Hubble expansion rate and they can be treated as separate species. The presence of small quantities of \( D \) and \( ^{3}He \) will not affect the evolution of \( ^{7}Li \). Thus, we have the system of equations for the average velocities \( V_a \) of individual species,

\[
\frac{\partial V_a}{\partial t} \approx g - \nabla P_a + \frac{q_a}{m_a} E - \sum_b \frac{V_a - V_b}{\tau_{ab}} + \tau_{ab}^{\text{ext}} / m_a . \tag{1}
\]

In these equations, \( g \) is the gravitational acceleration, \( E \) is the electric field strength, \( P_a, \rho_a = m_a n_a \), and \( q_a \) are the partial pressure, mass density, and the electric charge for different species respectively. For the electromagnetic effects we assume the tight charge coupling approximation. The \( V_a - V_b \) diffusion term is governed by the diffusion coefficients \( \tau_{ab}^{-1} \)

\[
\tau_{ab}^{-1} = (3T_m b)^{-1} \times \mu_{ab}^2 n_b (\sigma_{ab} v^3), \tag{2}
\]

that are in turn determined by the transport cross sections \( \sigma_{ab} \), averaged over the microscopic velocity distribution. We use lower and upper case to distinguish between thermal \( v \) and diffusional \( V \) velocities. \( \mu_{ab} \) is reduced mass and \( T \) is the temperature of the matter species.

Finally, the last term in \([1]\) accounts for the possibility of additional external forces, such as radiation pressure, Lorentz force, etc., with dependence on species index \( a \). However, we take \( \tau_{ab}^{\text{ext}} = 0 \) for the rest of this analysis.

In the next step, we solve Equations \([1]\) in the regime of small density perturbations, \( \delta \rho_a / \rho_a \ll 1 \), and specifically consider a sub-Jeans regime for baryons, that are forced inside an already formed dark matter halo by its gravitational acceleration \( g \). For a realistic choice of parameters \( 1/\tau \rightarrow \infty \) is a good zeroth order approximation, leading to vanishing \( \dot{V}_i \), in hydrostatic equilibrium. Thus, assuming that initial distribution of elements is uniform, one gets a relation between gradients of individual pressure contributions and \( g \) (see, e.g. \([7]\)),

\[
\nabla P_a / \rho_a = \sum b m_b n_b g = m / m_a g, \tag{3}
\]

and the quasi-static version of Eq. \([1]\) reduces to a set of algebraic equations,

\[
g \left( 1 - \frac{m}{m_a} \right) + \frac{q_a}{m_a} E - \sum_b \frac{V_a - V_b}{\tau_{ab}} = 0. \tag{4}
\]

We assume 25% mass fraction of \(^{4}He \) so that \( n_{^{4}He}/n_H = 1/12 \) and \( m_r \approx (4m_p + 12m_p)/(1 + 12) = \frac{5}{13} m_p \). The reduction of \( m_r \) due to ionized fraction can be safely neglected.

For the two dominant neutral components, hydrogen and helium, the solution is readily found:

\[
\frac{V_{He} - V_H}{\tau_{HeH}} = g \left( 1 - \frac{m_r}{m_{He}} \right) = \frac{9}{13} g. \tag{5}
\]

One can see that \( V_{He} - V_H \) is parallel to \( g \), as expected.

We now turn to the diffusion of charged particles and account for \( E \) in the equations. Solving them for electrons with the use of \([3]\) and \( m_e \ll m_{atom} \), one can easily find

\[
E \simeq -\nabla P_e / (en_e) = -(\overline{m}/e) g, \quad \text{where } e \text{ is the positron charge.}
\]

Carrying this to the equation for protons (or \( H^+ \)), we get the solution for the relative diffusion velocity:

\[
(V_p - V_H) \times \left( \frac{1}{\tau_{pH}} + \frac{1}{\tau_{pHe}} \right) = -g \left( \frac{m_r}{m_p/2} - 1 \right)
\]

\[
- \left( 1 - \frac{m_r}{m_{He}} \right) \frac{\tau_{HeH}}{\tau_{pHe}} = -g \left( \frac{9}{13} - \frac{9n_{HeH}}{13\tau_{pHe}} \right), \tag{6}
\]

using Equation \([5]\). The appearance of \( m_p/2 \) in this equation is easy to interpret: the effect of the EM force is such that the motion of \( e \) and \( p \) is tightly coupled together, so that their effective mass per particle is \( m_p/2 \), and indeed lighter than \( m_r \). This results in the diffusion of both \( e \) and \( H^+ \) against the direction of the gravitational acceleration, if helium contribution is negligible.

We are now ready to include the diffusion of Lithium, using already found solutions for \( V_p - V_H \) and \( V_{He} - V_H \). The general expression is given by

\[
(V_{Li} - V_H) \times \left( \frac{1}{\tau_{LiH}} + \frac{1}{\tau_{LiHe}} + \frac{1}{\tau_{LiP}} \right)
\]

\[
= -g \left\{ \frac{2m_r}{m_{Li}} - 1 - \left( 1 - \frac{m_r}{m_{He}} \right) \frac{\tau_{HeH}}{\tau_{LiHe}} \right. \frac{m_r}{m_p} - 1 - \left( 1 - \frac{m_r}{m_{He}} \right) \frac{\tau_{HeH}}{\tau_{pHe}} \frac{1}{\tau_{LiP}} + \frac{2m_r}{m_{p}} \right\}. \tag{7}
\]

It turns out that, to a good approximation, we can neglect the helium contribution, \( n_{He}/n_H \rightarrow 0 \), thus \( \tau_{pHe}^{-1} \rightarrow 0, m_r \rightarrow m_p, \) and the cumbersome expressions in Equations \([4,6]\) simplify to

\[
n_{He}/n_H \rightarrow 0 \text{ limit : } \frac{V_p - V_H}{\tau_{pH}} = -g; \tag{8}
\]

\[
(V_{Li} - V_H) \left( \frac{1}{\tau_{LiH}} + \frac{1}{\tau_{LiP}} \right) = g \left( \frac{5}{7} - \frac{\tau_{pHe}}{\tau_{LiP}} \right), \tag{9}
\]

where in the last formula we approximated \( m_{Li} = 7m_p \). The direction of the lithium diffusional velocity is far from obvious: it depends on the competition of the two terms on the r.h.s. of Equation \([8]\), and if the friction relative to \( p \) wins (i.e. small \( \tau_{lip} \) limit), the motion of \( Li^+ \) ions will trace the motion of ionized fraction of hydrogen gas. Indeed, Eq. \([8]\) reduces to \( (V_{Li} - V_H)/\tau_{pH} = -g, \)
or $V_{\text{Li}} = V_p$, if $\tau_{\text{Li}^{-1}}$ is the largest parameter. We now need additional input with actual size of $\tau_{ab}^{-1}$.

The scattering of $^4\text{He}$ on $p$ has been calculated in \cite{11}. The value of the transport cross section in the range of energies we are interested in, and its weighted average over the Maxwellian velocity distribution is given by

$$\sigma_{\text{HeH}} \simeq 100a_B^2; \quad \langle \sigma_{\text{HeH}} v^3 \rangle \simeq (32/\pi)^{1/2} \left( \frac{T}{\mu_{14}} \right)^{3/2} \sigma_{\text{HeH}},$$

where $T$ is the temperature of the baryonic fluid, $a_B = 1/(\alpha m_e)$, is the Bohr radius, and $\mu_{14} = 4m_p/5$. The cross sections of a singly-charged ion on a neutral atom can be approximated as $\sigma_{ab} \simeq 2.2\pi^{2} \left( \frac{\alpha_{\text{pol}}(b)}{2\pi} \right)^{1/2}$ \cite{12}, leading to

$$\langle \sigma_{ab} v^3 \rangle \simeq 20\pi a_B^2 \frac{Ry^{1/2}T}{\mu_{ab}} \left( \frac{\alpha_{\text{pol}}(b)}{\alpha_{\text{pol}}(\text{He})} \right)^{1/2},$$

where $\alpha_{\text{pol}}(b)$ is the atomic polarizability of the neutral species $b$: $\alpha_{\text{pol}}(\text{He}) = \frac{3}{2}a_B^2$ and $\alpha_{\text{pol}}(\text{He}) = 1.37a_B^2$. Ry stands for the hydrogen binding energy, $\text{Ry} \equiv \alpha^2m_e/2 \simeq 13.6$ eV. We should note that $p$-H scattering is in practice a more complicated process due to the identical nature of the nuclei involved, and a far more elaborate treatment of the $p$-H cross section can be found in \cite{13}. However, for the accuracy of our discussion, we shall approximate it with Eq. \cite{10}. Finally, and most importantly, the $p$-$\text{Li}^+$ scattering is given by the Rutherford formula,

$$\langle \sigma_{\text{Lip}} v^3 \rangle = \frac{8\pi^{2}a^2}{(2T)^{1/2} \mu_{17}} \times \ln \Lambda = 16\sqrt{2\pi}a_B^{2} \frac{\text{Ry}^{2}\ln \Lambda}{T^{1/2} \mu_{17}^{3/2}}$$

where $\mu_{17} = \frac{7}{8}m_p$, and $\ln \Lambda$ is the Coulomb logarithm. For the conditions of primordial plasma after the recombination, its value is large, in $\Lambda \sim 40$, and weakly dependent on temperature. Because of the long-range nature of the EM force, Eq. \cite{11} exhibits strong enhancement by $(\text{Ry}/T)^{3/2}/\ln \Lambda$ at small velocities/low temperatures.

We are now ready to determine the sign of the r.h.s. bracket in the simplified formula \cite{8}:

$$\frac{5}{7} - \frac{\tau_{\text{Lip}}}{\tau_{\text{Li}}^p} \simeq \frac{5}{7} - 300 \times \frac{X_e}{10^{-3}} \times \frac{\ln \Lambda}{40} \times \left( \frac{\text{Ry}}{T_{\text{baryon}}} \right)^{3/2} < 0,$$

where the abundance of free protons in the primordial plasma is the same as the electron ionization fraction $X_e$. It is easy to see that for the cosmological parameters between recombination and re-ionization, the expression \cite{12} is negative. In Figure 1, we plot the the positivity condition on $X_e$-redshift plane, assuming standard relations between $T$, photon temperature $T_{\gamma}$ and redshift $z$. The separatrix stays firmly below cosmological $X_e(T)$ at all redshifts. One can see that even tiny values of $X_e$ would lead to a tight coupling of lithium to $H^+$, resulting in outward diffusion of lithium. We can also quantify

$$\text{FIG. 1. Post-recombination ionization fraction } X_e(T) \text{ (black line) and the separatrix for the direction of } V_{\text{Li}} - V_H \text{ relative to } g. \text{ Above the gray line Eq. } \text{[12]} \text{ holds, and since it stays always below the black curve, lithium diffuses "out", leading to } [\text{Li}/H]_{\text{grav min}} < [\text{Li}/H]_{\text{SBBN}}.$$  

the ratio of relative velocities,

$$\frac{|V_{\text{Li}} - V_H|}{|V_p - V_H|} \simeq 1 - \frac{12}{7} \tau_{\text{Lip}} - 1 \approx 10^{-2},$$

which are different only at $O(\%)$ level. Conclusions of Eqs. \cite{12} and \cite{13} are due to large size of the Rutherford cross section that overcomes the rarity of $H^+$. Inclusion of He into this analysis does change the conclusions somewhat; while Li$^+$ remains tightly bound to H$^+$, the outward diffusion of ionized H$^+$ is no longer guaranteed. We find that for most of the redshift of interest, $z > 30$, both $p$ and Li diffuse out of overdensities not changing the qualitative details of the simplified analysis.

Do we understand the magnitude and sign of possible $[\text{Li}/H]$ variations? While we have shown that, quite unexpectedly, the direction of lithium diffusion in the early Universe after the recombination is against local gravitational force, it is clear that it would be difficult to create variations in lithium abundance at $O(1)$ level. Let us assume to good accuracy that $1/\tau_{\text{Lip}}$ is the largest coefficient, so that motion of Li$^+$ and H$^+$ are spatially linked. Then, using the continuity equations we can tie the variation in lithium abundance that develops at redshift $z_f$ to the local halo density,

$$[\text{Li}/H]_{\text{SBBN}} - [\text{Li}/H]_{\text{halo}} \simeq - \int_{t_i}^{t_f} dt \frac{\nabla \cdot \mathbf{g}}{1/\tau_{\text{PH}}}$$

$$= \int_{t_i}^{t_f} dt \frac{4\pi G \rho_{\text{halo}}}{\tau_{\text{PH}}}$$

$$\simeq 1 \times 10^{-2} \left( \frac{\Delta}{200} \right) \left( 1 + \frac{z_f}{20} \right)^{-3/2}.$$  

Here $\mathbf{p}$ is the average matter density, while $\rho_{\text{halo}}$ is the mass density of the halo, which is presumably con-
Supersonic halo mergers lead to turbulence which further suppresses the diffusion. Furthermore, the ionization fractions may differ from the cosmological values at significant gas overdensities. On the other end, for smaller haloes the supersonic relative velocities of dark matter and baryons suppresses diffusion, except within a small fraction of cosmic volume \[15\]. Thus, only careful hydrodynamic simulations of early star formation, which include diffusion effects, will be able to confirm the real(istic) magnitude of lithium depletion in population II and III stars.

Finally, we would like to stress that perhaps our most interesting and novel result is that lithium remains closely tied to ionized fraction of the gas. Therefore, any additional forces \(f_s\) that act on neutral and charged components differentially, could play a role in creating variations in lithium abundance. Interesting candidates for creating such forces are radiation pressure/stellar winds from first stars, and possibly primordial magnetic fields. This whole scope of issues deserves close attention due to the continuing interest in the lithium problem.

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