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ABSTRACT

My report on some "isomer intuition" network calculations with the ^{85}Kr ground and isomeric state.

1. INTRODUCTION

I ran several network calculations to test the network with transitions from the ground to isomeric state and back for ^{85}Kr in a temperature-varying environment. I report here.

2. THE CALCULATIONS

I added to the network code a thermodynamic trajectory module to allow for sinusoidally varying temperature and density. The input parameters to the routine are the initial temperature and density, the oscillation timescale, and the fractional amplitude variation of the density. The density varied with the temperature as $\rho \propto T_9^3$.

Figure 1 shows the T_9 versus time for a calculation with initial $T_9 = 0.2$, an oscillation timescale of 10 seconds, and a fractional density variation of 50%. In all, I ran five calculations. They were: 1) a calculation at constant $T_9 = 0.2$ (achieved by making the density variation amplitude equal to zero), 2) a calculation at constant $T_9 = 1$, 3) a calculation at constant $T_9 = 3$, 4) the calculation shown in Fig. 1, and 5) a calculation similar to that in Fig. 1 but with initial $T_9 = 1$. All calculations had initial density $\rho = 10^3$ g/cc. In all cases the network consisted simply of n, p, and the ground and isomeric ensembles of ^{85}Kr (the network requires the neutrons and protons in general to compute binding energies). The only reactions present were the reactions between the ground and isomeric ensembles. I computed the ground to isomer transition rate from the isomer to ground rate and detailed balance. To do so, I used the ground and isomeric ensemble partition functions provided by Wendell.

I carried out the calculations on my laptop using a Docker image I built. Plots were made with our python library wnutils. I encapsulated all this in a script *isomer_intuition.sh*.

3. RESULTS

The first calculation was for constant $T_9 = 0.2$. Figure 2 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus time. Mass transfers slowly from the ground to the isomer ensemble on a $\sim 10^5$ second timescale. Eventually, the system reaches equilibrium.

The second calculation was for constant $T_9 = 1$. Figure 3 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus time. Mass transfers quickly from the ground to the isomer ensemble and reaches equilibrium in less than a microsecond. The figure also shows the equilibrium level the system would reach if the equilibrium were only that of the ground state and isomer state themselves, not including the ensemble. The two equilibria are nearly the same, which shows the ensemble populations are dominated by the ground and isomer states themselves.

The third calculation was for constant $T_9 = 3$. Figure 4 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus time. Here the transition to equilibrium occurs very quickly. Also it is clear that the equilibrium from just the ground and isomer states is quite different from that in the ensembles. This shows that that a significant fraction of the ensemble abundances are in the upper-lying states.

The fourth calculation was for varying T_9 with initial $T_9 = 0.2$ (the calculation shown in Fig. 1). Since the timescale for nuclei to transition from the ground to isomeric ensemble (and back) is longer than the oscillation timescale, the

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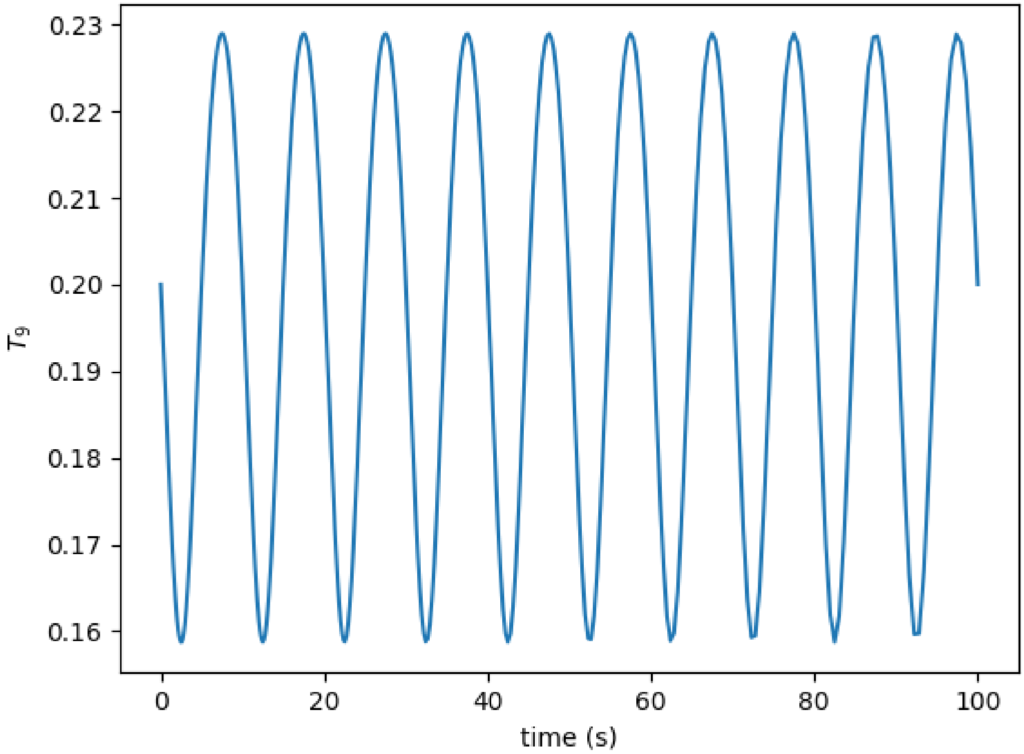

Figure 1. The temperature vs. time for a varying calculation.

system "pumps" mass into the isomer. Figure 5 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus time. Figure 6 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus T_9. Mass moves to the isomer most rapidly when the temperature is near its peak, while at lower temperature the mass is simply trapped in either state since the transition timescales are much less than the temperature oscillation timescale.

The last calculation was for varying T_9 with initial $T_9 = 1$. Since the timescale for nuclei to transition from the ground to isomeric ensemble (and back) is shorter than the oscillation timescale, the system quickly achieves equilibrium and maintains it throughout the variations. Figure 7 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus time. Figure 8 shows the $^{85}\mathrm{Kr}_m$ mass fraction versus T_9.

4. CONCLUSION

The calculations agree with (at least) my intuition in how the system should behave with time varying density and temperature. The network codes and python routines are in place. My main todos are 1) to finish adding routines to the python library to modify the nuclear and reaction input (to make incorporation of the isomer data easier) and 2) to modify our flow diagram code to accommodate isomers. I should be able to make significant progress on both of these tasks over the next month or so. I also look forward to running with a set of trajectories.

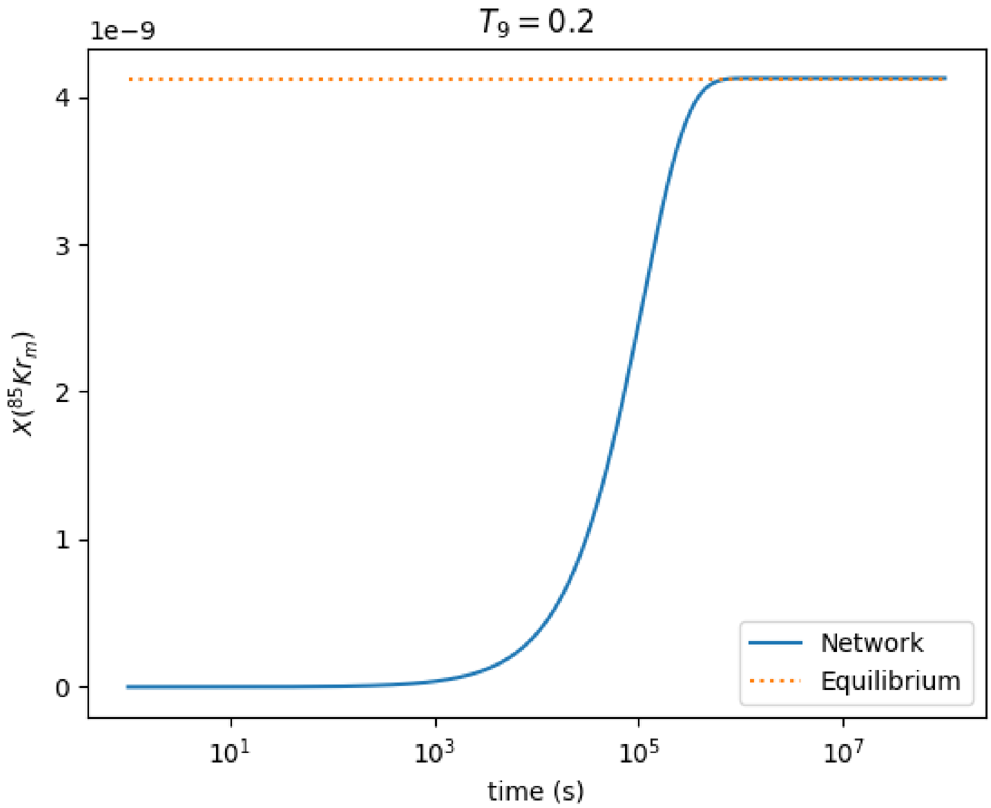

Figure 2. The $^{85}\mathrm{Kr}_m$ mass fractions vs. time.

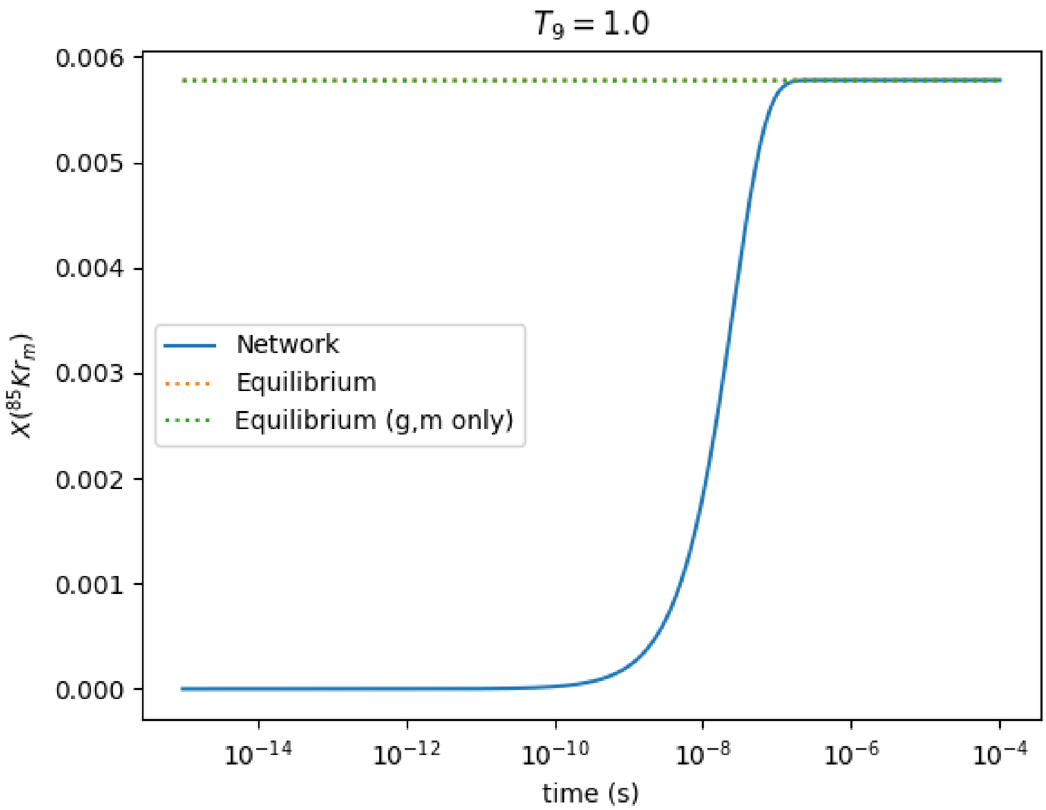

Figure 3. The $^{85}\mathrm{Kr}_m$ mass fractions vs. time.

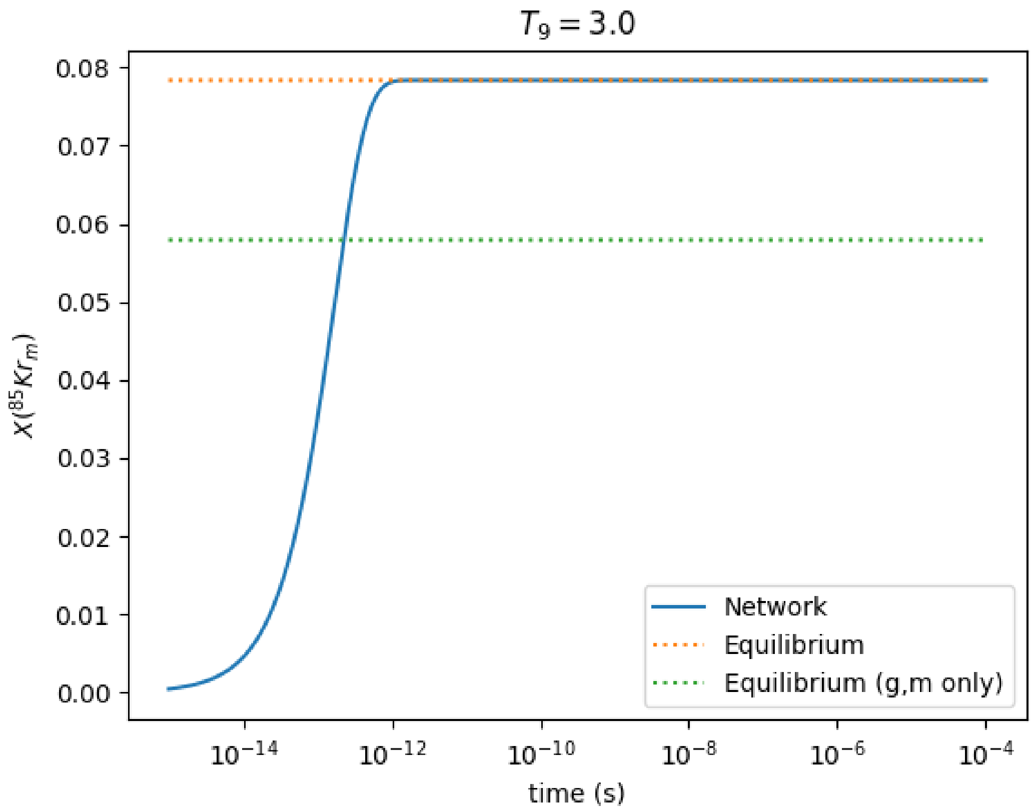

Figure 4. The $^{85}\mathrm{Kr}_m$ mass fractions vs. time.

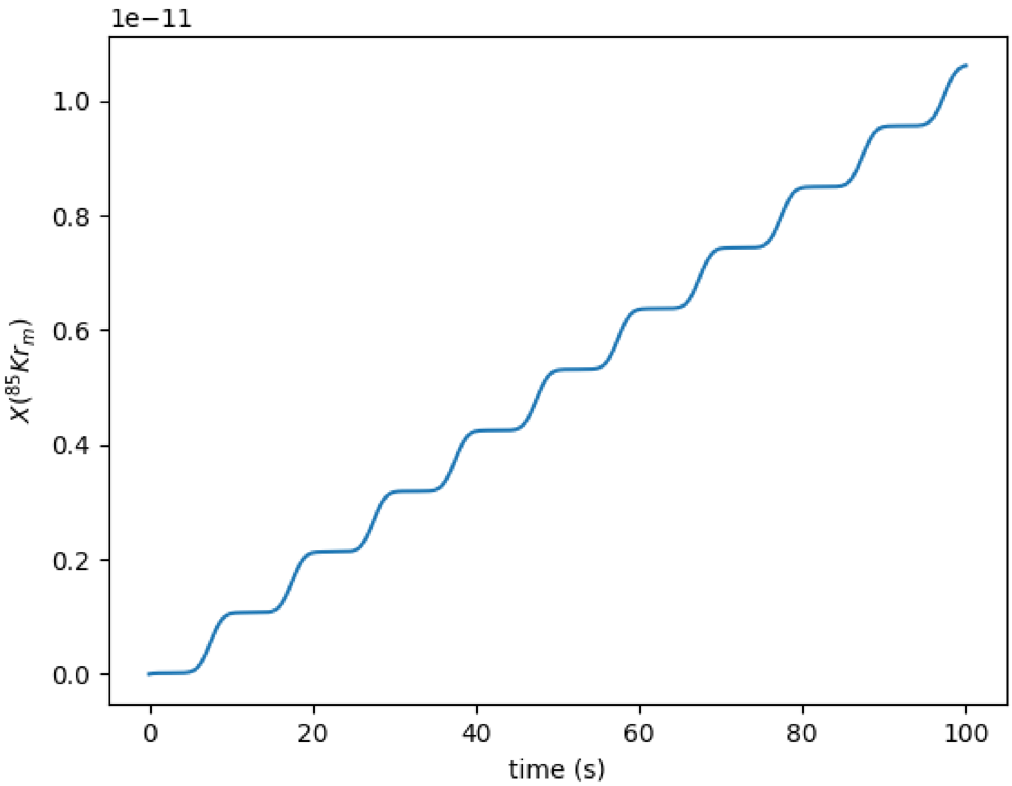

Figure 5. The ^{85}Kr$_m$ mass fractions vs. time.

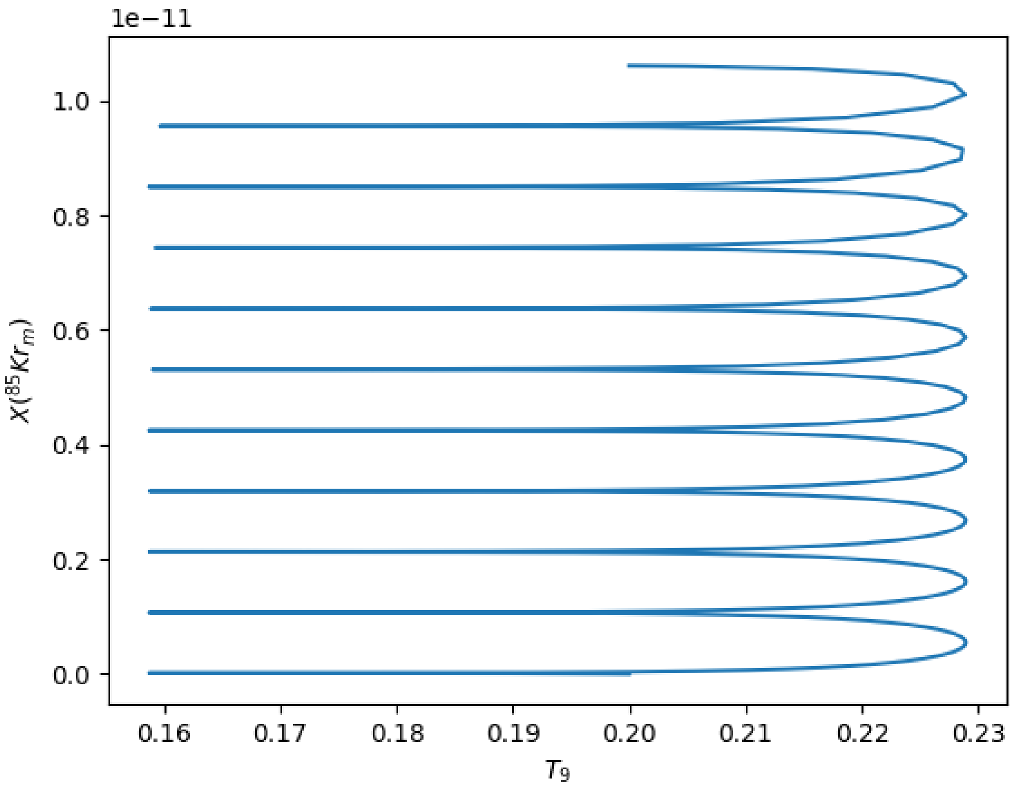

Figure 6. The $^{85}\mathrm{Kr}_m$ mass fractions vs. T_9.

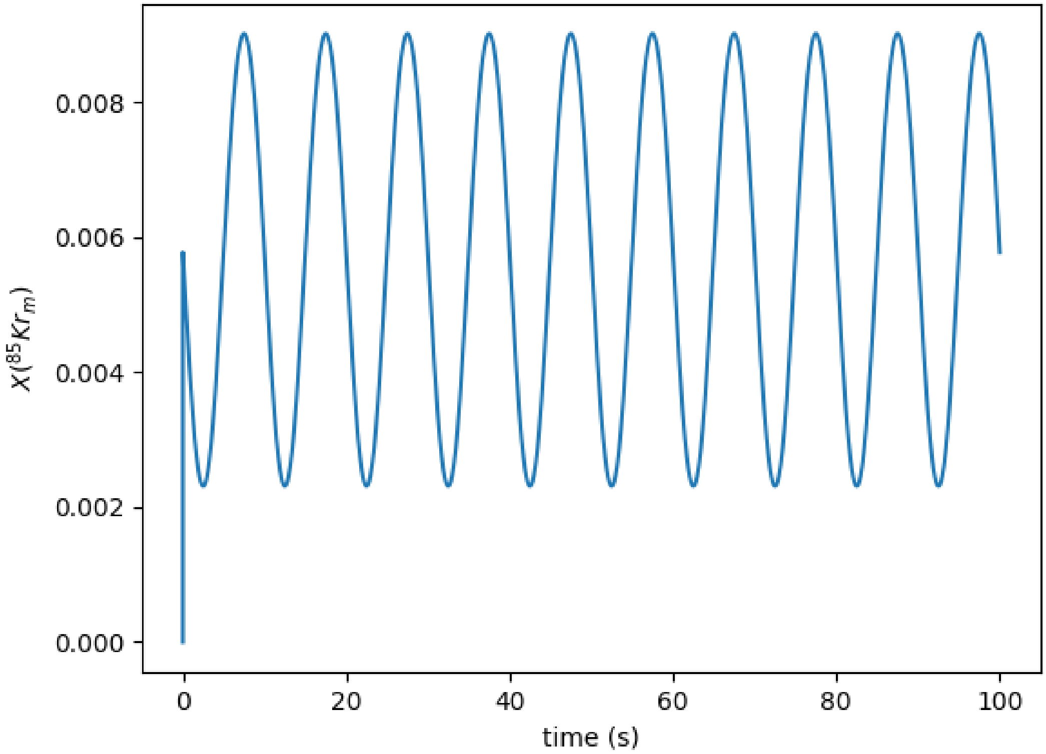

Figure 7. The $^{85}\mathrm{Kr}_m$ mass fractions vs. time.

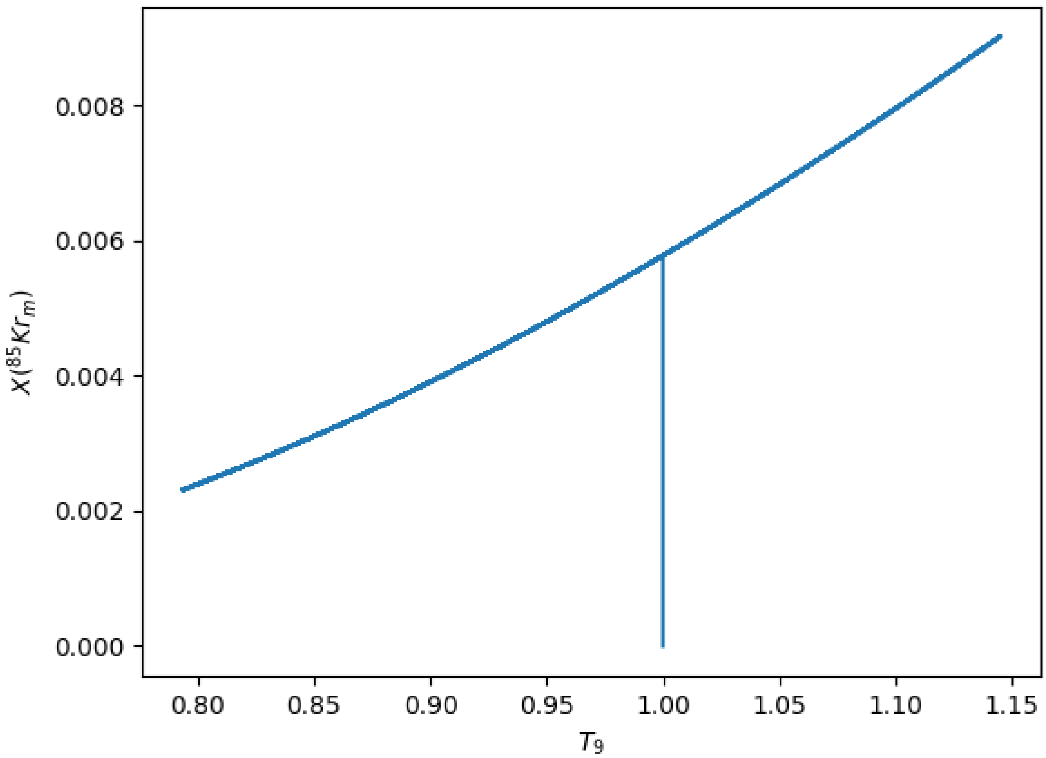

Figure 8. The $^{85}\mathrm{Kr}_m$ mass fractions vs. T_9.