CLUSTERING EFFECTS IN THE EQUATION OF STATE ON NUCLEAR MATTER

A Thesis

by

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ABSTRACT

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In Nuclear AstroPhysics, clustering refers to the process by which atomic elements, known as nuclei, are formed from pre-existing nucleons such as protons and neutrons. This process called nucleosynthesis, is thought to occur under the following scenarios: Big Bang nucleosynthesis, Stellar nucleosynthesis, explosive nucleosynthesis and nucleosynthesis derived from fragmentation processes in nuclear reactions. In the case of all except the latter, which deals with radioactive decay and fission (the dissociation of larger nuclei into smaller ones), nucleosynthesis is predominantly the result of fusion, which is the creation of larger nuclei from smaller ones.

To date, our current understanding of nuclei formation has crucial limitations, which is due to the complexity of stellar-nucleosynthesis and related processes. To overcome this gap in our understanding, of particular note and interest is explosive nucleosynthesis which involves the r-process, rp-process, s-process and p-process which are theorized to be the means by which elements more massive than iron are formed.

Furthermore, the processes governing the different types of nucleosynthesis are additionally delineated by the relative rate at which nuclei formation occurs - which ranges from very rapidly in the order of seconds, to extremely long in the order of centuries, depending on the element and process in question. In attempting to reach an understanding of these

processes, an additional caveat appears in that most of these processes are theorized to occur near the end of life of star - i.e. in a supernova event which is thought to supply both the high energy, temperatures and pressure with which to form these heavy nuclei. Consequently, neutron stars, which are highly dense stellar remnants of core-collapse supernova events, are potential candidates whose environments and existence are theorized to provide the ideal physical characteristics for the aforementioned processes hence explaining the formation of nuclei heavier than iron in neutron star mergers events.

Although similar has work done on clustering in determining the physics, structure and evolution of neutron stars and their associated equations of state, it is not well known how such considerations derived from statistical physics affects heavy nuclei formation.

Subsequently, one means of understanding these processes is to approach everything from a rigorous thermodynamical treatment. However, as nuclear species can vary up in relative occupied volumes, we must account for the thermodynamic potential variance due to the occupied nuclear volume for interacting species in our treatment. And, as that variance could be potentially large, this fact violates the core tenet of the ideal gas law as we can no longer treat the particles as point particles but rather as particles with definite and non-infinitesimal volumes - which means that we can assert that the particles affect the occupied volume of the space in which they interact and occupy. Consequently, any treatment and inclusion of the ideal gas law and any derived thermodynamical potentials cannot be used or applied as the physics of those treatments are inapplicable in this situation. What this means is that for us to perform any useful calculation, we must account for the occupied particle species volumes in any thermodynamical potential - something that has to be derived and verified from scratch with many possible alternative methods.

This idea of volume isolation or more accurately, exclusion, is called excluded-volume mechanism (excluded-volume can be thought to be the occupied volume minus the total volume occupied by all the particles), an approach that is fairly common in BioPhysics, but one that is not so common in nuclear astrophysics, with particular attention to how such an approach affects the formation of nuclei and the associated equations of state.

To determine the effects, if any, that excluded volume may have on the equation of state, we begin by applying excluded-volume mechanism on classical thermodynamics and associated thermodynamical potentials by modifying the standard methodology of considering the non-relativistic energetics of non-interacting particles from a purely statistical mechanical approach, known as a Maxwell-Boltzmann statistics. Having considered excluded-volume statistically, we can derive thermodynamical potentials of interest such the reduced Gibb's Free Energy, which can be used to formulate a rudimentary equation of state.

But, as this approach doesn't consider readily apparent physics that dominate neutron stars such as quantum mechanics, we have to extend this treatment even further by such an inclusion (via energy degeneracy and the inclusion of bound and occupied states of the particles), in addition to angular momentum and relativistic effects to create a more realistic physical model which can be applied and used in determining the associated equations of state and how nuclei formation is affected as a result.

Summarily, as the thermodynamics determines the inter-particle distance due to arguments based on particle energy, degeneracy, chemical potential, etc., it is our hope that such a treatment will not only prove to be definitive, but useful in constraining our understanding of these processes having utilized the relatively unexplored mechanism of excluded-volume, in its determination of the equation of state and how that affects nuclei formation in neutron stars.

This work has been done in collaboration with the nuclear astrophysics group of Catania, Sicily, under the leadership of Prof. Spitaleri and with Dr. Stefan Typel from GSI, Darmstadt, Germany.

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STATISTICS AND THERMODYNAMICS OF PARTICLES WITH FINITE SIZE

Introduction

If we consider a system composed of different particle species i with particle numbers N_i in a volume V at some temperature T, we can denote the particle densities as

$$n_i = \frac{N_i}{V}, \tag{1.1}$$

where we assume that every particle species i has a degeneracy factor g_i and a chemical potential μ_i for particles with rest mass m_i. The energy of a particle is denoted by E_i and includes the rest mass. We will use canonical and grand canonical statistical ensembles and different particle statistics in the following.

More specifically, according to Greiner et al. (1999), the canonical ensemble is suited for systems in a heat bath with a given T, V and N. On the other hand, the grand canonical - also called the macrocanonical ensemble - describes open systems where heat and particles are exchanged with the surroundings.

Classical Excluded Volume Mechanism

If we also assume Maxwell-Boltzmann statistics for noninteracting particles with nonrelativistic energy (in units of $\hbar = c = k_B = 1$); we have

$$E_i(k) = \frac{k^2}{2m_i} + m_i, \tag{1.2}$$

that depends on the particle momentum k.

According to (Greiner et al., 1999, p. 187 - 189), Maxwell-Boltzmann statistics assumes that for a given temperature, particles are distinguishable and that quantum mechanics plays a negligible role. These two assumptions while seemingly valid at first, create a number of problems depending on the particles and system.

This indistinguishability is "corrected" by the inclusion of the Gibbs factor $1/N!$ - as noted in (Greiner et al., 1999, p. 133), which removes contradictions arising from the assumption that particles are distinguishable. And, depending on the particles and system in question, we will show that quantum statistics will have to be included where we will introduce Planck's constant, h and other physical considerations.

Given this information, it is more appropriate to consider the free energy of the system - which is energy that can be used to perform work (that includes the contributions of rest mass), in contrast to the total energy, E. More specifically, if we begin with an ideal gas approximation with constant temperature and volume, the free energy in question is actually the Helmholtz energy. (Huang, 2001, p. 38)

To begin our derivations, we use the definitions for the Helmholtz free energy

$$F(T, V, N) = U - TS, \tag{1.3}$$

$$dF = -p\mathrm{d}V - S\mathrm{d}T + \sum_i \mu_i \mathrm{d}N_i, \tag{1.4}$$

and the Gibbs free energy

$$G(T, p, N) = U - TS + pV, \tag{1.5}$$

$$dG = V\mathrm{d}p - S\mathrm{d}T + \sum_i \mu_i \mathrm{d}N_i. \tag{1.6}$$

Physically, the meaning of the Helmholtz free energy is that of work done on the system plus heat loss from it, under constant pressure and entropy. The Gibbs free energy is the same, but for constant volume. In both cases, one adds the energy required to change the particle number. μ, the chemical potential, is the energy change by adding one particle to the system.

And, to consider more realistic physical systems, if we apply the Gibbs correction factor (to "correct" contradictions arising from the initial assumption that for Maxwell-Boltzmann statistics all particles are distinguishable), on an ideal gas and consider phase space volume elements of size h^{3N} to determine the mean number of states per energy interval, we can use the "absolute entropy" of an ideal gas, also known as the Sackur-Tetrode equation, from which in (Greiner et al., 1999, p. 137 - 139), we can develop a more specialized form of the Helmholtz free energy to determine thermodynamic variables and potentials of interest

$$S(U,V,N) = Nk_B \left[\frac{5}{2} + \ln \left\{ \frac{V}{N} \left(\frac{4\pi m U}{3N} \right)^{3/2} \right\} \right]. \tag{1.7}$$

Notably, we observe that h, Planck's constant appears in the Sackur-Tetrode equation - which comes from a "pseudo-quantum mechanical" counting of the number of micro-states where "the total energy is determined by the $3N$ quantum numbers of the occupied states" (Greiner et al., 1999, p. 135)

$$U = E = \frac{h^2}{8mL^2} \sum_{i=1}^{3N} n_i^2 \tag{1.8}$$

Then, solving for the internal energy, U

$$U(S,V,N) = \frac{3h^2 N^{5/3}}{4\pi m V^{2/3}} \exp\left\{ \frac{2S}{3Nk_B} - \frac{5}{3} \right\}, \tag{1.9}$$

the variation of the internal energy under constant pressure and temperature is given by (Greiner et al., 1999, p. 140)

$$\mathrm{d}U = T\mathrm{d}S - p\mathrm{d}V + \mu\mathrm{d}N. \tag{1.10}$$

Hence,

$$T = \left.\frac{\partial U}{\partial S}\right|_{N,V} = \frac{2}{3Nk_B}U \rightarrow U = \frac{3}{2}Nk_BT, \tag{1.11}$$

$$-p = \left.\frac{\partial U}{\partial V}\right|_{S,N} = -\frac{2}{3V}U \rightarrow U = pV = Nk_BT, \tag{1.12}$$

$$\mu = \left.\frac{\partial U}{\partial N}\right|_{S,V} = U\left(\frac{5}{3N} - \frac{2S}{3N^2k_B}\right) = k_BT\ln\left\{\frac{N}{V}\left(\frac{h^2}{2\pi mk_BT}\right)^{3/2}\right\}. \tag{1.13}$$

Now, we can define a specific form the Helmholtz free energy using eqs. (1.7) and (1.11)

$$F = U - TS = Nk_BT\left[\ln\left\{\frac{N}{V}\left(\frac{h^2}{2\pi mk_BT}\right)^{3/2}\right\} - 1\right]. \tag{1.14}$$

The thermal wavelength - or the de Broglie wavelength for a gas in equilibrium at temperature, T as shown (Huang, 2010, p. 195) - is defined as (here we restore $\hbar$ and k_B to explicitly show their dependence)

$$\lambda_i = \sqrt{\frac{2\pi\hbar^2}{m_i k_B T}}. \tag{1.15}$$

Then, setting $\hbar = k_B = 1$ (as done previously), we obtain

$$\lambda_i = \sqrt{\frac{2\pi}{m_i T}}. \tag{1.16}$$

Using eqs. (1.16) and (1.14) the free energy becomes

$$F = U - TS = N k_B T \left[\ln\left(\frac{N}{V} {\lambda_i}^3 \right) - 1 \right]. \tag{1.17}$$

The degeneracy increases the number of possible states in the system (similar to increasing the volume). Hence, we can write (note that the i subscript here means the particle in question - e.g. $i = n$)

$$F(T, V, N_i) = \sum_i N_i \left[T \ln\left(\frac{N_i {\lambda_i}^3}{g_i V} \right) - T + m_i \right], \tag{1.18}$$

Noting the presence of $\hbar$ in the thermal wavelength suggests that quantum mechanics is important to the calculation of the Helmholtz free energy. However, with this consideration we immediately violate one of the requirements for Maxwell-Boltzmann statistics (that quantum mechanical effects are considered to be minuscule such that they can be neglected altogether).

This means that with the introduction of h we make the assertion that while Maxwell-Boltzmann statistics are a good starting point to describe the physical constraints, we assume that quantum mechanical effects will have a part to play in the overall behavior and description of the system because of the nature of the particles in question; and, the scale of the overall interaction distances - as the average inter-particle distance has to be compared to the deBroglie wavelength of the particles. Notably, when the thermal wavelength is much smaller than the inter particle distance, we recover the classical behavior. However, it should be noted that as this treatment is not entirely quantum mechanical derived, it is actually semi-classical.

Additionally, we use λ - the deBroglie wavelength - in eq. (1.18),

$$\lambda = \frac{h}{\sqrt{2mE_K}}, \tag{1.19}$$

where E_K is the average kinetic energy of the thermal particles. Indeed, using $E_K \approx k_B T$, we recover eq. (1.15).

Furthermore, we note that the natural variables here are the temperature T, the volume V and the particle numbers N_i. Hence, we can then define the chemical potentials of the particles as

$$\mu_i = \left.\frac{\partial F}{\partial N_i}\right|_{T,V,N_{j\neq i}} . \tag{1.20}$$

Similarly, the entropy is given by eq. 3.37 of (Huang, 2001, p. 37)

$$S = -\left.\frac{\partial F}{\partial T}\right|_{V,N_i} . \tag{1.21}$$

And, in like fashion the pressure is obtained from

$$P = -\left.\frac{\partial F}{\partial V}\right|_{T,N_i} . \tag{1.22}$$

We begin determining the values of these potentials by using the relationship

$$\frac{d}{dx}\left[\alpha\, x \ln\left(\frac{x}{\beta}\right)\right] = \alpha + \alpha \ln\left[\frac{x}{\beta}\right], \tag{1.23}$$

hence, we can then find

$$\begin{aligned}\mu_i &= \left.\frac{\partial F}{\partial N_i}\right|_{T,V,N_{j\neq i}}\\ &= T + T\ln\left(\frac{N_i{\lambda_i}^3}{g_i V}\right) - T + m_i\\ &= T\ln\left(\frac{N_i{\lambda_i}^3}{g_i V}\right) + m_i. \end{aligned} \tag{1.24}$$

Similarly, for the entropy,

$$\begin{aligned} S &= -\left.\frac{\partial F}{\partial T}\right|_{V,N_i} \\ &= -\sum_i N_i \left[\ln\left(\frac{N_i{\lambda_i}^3}{g_i V}\right) - \frac{5}{2}\right], \\ &= \sum_i N_i \left[\frac{5}{2} - \ln\left(\frac{N_i{\lambda_i}^3}{g_i V}\right)\right], \end{aligned} \tag{1.25}$$

where we have used the relationship

$$\frac{d}{dT}\left(\alpha T\left[\ln\left[\frac{T^{-3/2}}{\beta}\right] - T\right]\right) = -\frac{5\alpha}{2} + \alpha\ln\left[\frac{T^{-3/2}}{\beta}\right]. \tag{1.26}$$

Finally, for the pressure, we get

$$P = -\left.\frac{\partial F}{\partial V}\right|_{T,N_i} = \sum_i N_i\frac{T}{V}. \tag{1.27}$$

Using these solutions, we can then obtain the total internal energy (eq. 4.52) in Greiner et al. (1999). Using the relation between the internal energy and the free energy

$$F = U - TS - \sum_i \mu_i N_i, \tag{1.28}$$

we get

$$\begin{aligned}
U(S,V,N_i) &= F(T,V,N_i) + TS = TS - pV + G \qquad (1.29)\\
&= T\sum_i N_i\left[\frac{5}{2} - \ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right)\right] - V\left(\sum_i N_i\frac{T}{V}\right)\\
&\quad +T\sum_i N_i\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right) + \sum_i N_i\, m_i,\\
&= T\sum_i N_i\left[\frac{5}{2} - \ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right)\right] - T\sum_i N_i\\
&\quad +T\sum_i N_i\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right) + \sum_i N_i\, m_i,\\
&= \sum_i N_i\left(\frac{5}{2}T - T + T\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right) - T\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right) + m_i\right),\\
&= \sum_i N_i\left(\frac{3}{2}T + m_i\right), \qquad (1.30)
\end{aligned}$$

where we used

$$\begin{aligned}
m_i &= \mu_i - T\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right).\\
\mu_i &= T\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right) + m_i. \qquad (1.31)
\end{aligned}$$

Therefore, we can write the energy in natural variables as

$$U(S,V,N_i) = \sum_i N_i\left[\frac{3}{2}T + \mu_i - T\ln\left(\frac{N_i{\lambda_i}^3}{g_iV}\right)\right]. \qquad (1.32)$$

And, using the grand canonical potential (a thermodynamic potential is a scalar function used to measure the state of a system), which describes the properties of an open system, i.e. a system with varying particle number, is defined as

$$\begin{aligned}\Omega(T,V,\mu_i) &= F(T,V,N_i) - \sum_i \mu_i N_i = -PV, \\ &= -V\left(\sum_i N_i \frac{T}{V}\right), \\ &= -\sum_i N_i T = -NT, \end{aligned} \tag{1.33}$$

where the natural variables of the different thermodynamic potentials are given as arguments in parentheses. Sometimes it is also useful to introduce the free energy density $f = F/V$, the internal energy density $u = U/V$, the entropy density $s = S/V$ and the grand canonical potential density $\omega = \Omega/V$.

Thermodynamic Potentials in Reduced Volume

A finite volume V_i can be introduced for every particle species such that the available volume for the motion is not V any more but the reduced volume.

We will use the raised symbol $\sim$ to indicate quantities in the description with excluded volume mechanism and generalizations.

$$\widetilde{V} = V - \sum_i N_i V_i. \tag{1.34}$$

Replacing V in eq. (1.18) by $\widetilde{V}$ one obtains the classical excluded volume mechanism in the free energy

$$\begin{aligned} \widetilde{F}(T, V, N_i) &= \sum_i N_i \left[T \ln \left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}} \right) - T + m_i \right], \\ &= \sum_i N_i \left[T \ln \left(\frac{N_i {\lambda_i}^3}{g_i V - g_i \sum\limits_j N_j V_j} \right) - T + m_i \right]. \end{aligned} \tag{1.35}$$

This approach is thermodynamically consistent since the natural variable of F is used in the formulation. Thus, using the developments in the section, we can then derive explicit expressions for the quantities μ_i, S, P, E and Ω in case of a gas with excluded volume.

The volume excluded chemical potential, $\widetilde{\mu}$ for each particle species i is

$$\begin{aligned}\widetilde{\mu}_i &= \left.\frac{\partial F}{\partial N_i}\right|_{T,V,N_{j\neq i}}, \\ &= T + T\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) - T + m_i + \sum_k N_k T\,\frac{g_k\sum_j \delta_{ij}V_j}{g_kV - g_k\sum\limits_j N_jV_j}, && (1.36)\\ &= T\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + m_i + TV_i\sum_k \frac{N_k}{V-\sum\limits_j N_jV_j}. && (1.37)\end{aligned}$$

Comparing this with the equation obtained for the chemical potential, $\mu_i = T\ln\left(N_i{\lambda_i}^3/g_iV\right) + m_i$, we see that the chemical potential for a reduced volume is larger.

Similarly, for the entropy

$$\begin{aligned}\widetilde{S} &= -\left.\frac{\partial F}{\partial T}\right|_{V,N_i}, \\ &= -\sum_i N_i\left[\ln\left(\frac{N_i(2\pi/m_iT)^{3/2}}{g_i\widetilde{V}}\right) - \frac{5}{2}\right], \\ &= \sum_i N_i\left[\frac{5}{2} - \ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right)\right]. && (1.38)\end{aligned}$$

Comparing this with the original value obtained for the entropy

$$S = \sum_i N_i\left[5/2 - \ln\left(N_i{\lambda_i}^3/g_iV\right)\right],$$

we see that the entropy is smaller for a reduced potential.

Finally, for the pressure,

$$\widetilde{P} = -\left.\frac{\partial F}{\partial V}\right|_{T,N_i} = T\frac{\sum_i N_i}{V - \sum_j N_j V_j}. \tag{1.39}$$

Comparing this against the value obtained previously for the pressure

$$P = \sum_i N_i \frac{T}{V},$$

we see that the pressure for reduced volume is higher. While seemingly unusual at first glance, this result is expected as we're working in a smaller volume with the same particle numbers, and system constraints. More specifically, since the Temperature has remained the same and we have a smaller volume, the pressure has to increase.

Combining all of these solutions, we can hence derive the total internal energy for a reduced volume

$$\begin{aligned}
\widetilde{U}(\widetilde{S},V,N) &= \widetilde{F}(T,V,N_i) + T\widetilde{S}, \\
&= T\widetilde{S} - \widetilde{p}V + \sum_i \widetilde{\mu}_i N_i, \\
&= T\sum_i N_i\left[\frac{5}{2} - \ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right)\right] - VT\frac{\sum_i N_i}{V - \sum_j N_jV_j} \\
&\quad + T\sum_i N_i \ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + \sum_i N_i\, m_i \\
&\quad + T\sum_i N_iV_i \sum_i \frac{N_i}{V - \sum\limits_j N_jV_j}, \\
&= \frac{5}{2}T\sum_i N_i - VT\frac{\sum_i N_i}{V - \sum_j N_jV_j} + \\
&\quad T\sum_j N_jV_j \sum_i \frac{N_i}{V - \sum\limits_j N_jV_j} + \sum_i N_i\, m_i, \\
&= \frac{5}{2}T\sum_i N_i - T\sum_i N_i\left[\frac{V}{V - \sum_j N_jV_j} - \frac{\sum_j N_jV_j}{V - \sum\limits_j N_jV_j}\right] \\
&\quad + \sum_i N_i\, m_i, \\
&= \sum_i N_i\left[\frac{3}{2}T + m_i\right]. \qquad (1.40)
\end{aligned}$$

Noting that

$$\begin{aligned}\widetilde{\mu}_i &= T\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + m_i + TV_i\sum_k \frac{N_k}{V-\sum\limits_j N_jV_j}. \\ &= T\left[\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + \frac{m_i}{T} + V_i\sum_k \frac{N_k}{V-\sum\limits_j N_jV_j}\right],\end{aligned} \tag{1.41}$$

we get

$$m_i = \widetilde{\mu}_i - T\left[\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + V_i\sum_k \frac{N_k}{V-\sum\limits_j N_jV_j}\right].$$

Hence, we can write the reduced volume energy as

$$\widetilde{U}(\widetilde{S},V,N) = \sum_i N_i\left[\frac{3}{2}T + \widetilde{\mu}_i - T\left(\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + V_i\sum_k \frac{N_k}{V-\sum\limits_j N_jV_j}\right)\right]. \tag{1.42}$$

Given this value, and comparing it against the value obtained previously for the internal energy, $E = \sum_i N_i\,(3T/2 + m_i)$, we observe that the total internal energy is identical to the internal energy in the regularly case, the ideal gas.

Similarly, for the grand canonical potential for a reduced volume

$$\begin{aligned}\widetilde{\Omega}(T,V,\mu) &= \widetilde{F}(T,V,N_i) - \sum_i \widetilde{\mu_i} N, \\ &= -\widetilde{P}V, \\ &= -TV\frac{\sum_i N_i}{V - \sum_j N_j V_j}, \\ &= -T\frac{\sum_i N_i}{1 - \sum_j n_j V_j}. \end{aligned} \tag{1.43}$$

Since

$$\widetilde{\mu_i} = T\ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}}\right) + m_i + TV_i \sum_k \frac{N_k}{V - \sum\limits_j N_j V_j},$$

we get

$$T\frac{\sum_i N_i}{1 - \sum_j n_j V_j} = \widetilde{\mu_i} - T\ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}}\right) - m_i,$$

or

$$-T\frac{\sum_i N_i}{1 - \sum_j n_j V_j} = T\ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}}\right) + m_i - \widetilde{\mu_i}. \tag{1.44}$$

Then we can write $\widetilde{\Omega}$ as a function of natural variables

$$\begin{aligned}\widetilde{\Omega}(T,V,\widetilde{\mu}) &= \widetilde{F}(T,V,N_i) - \sum_i \widetilde{\mu}_i N \\ &= -T\frac{\sum_i N_i}{1-\sum_j n_j V_j} \\ &= T\ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}}\right) + m_i - \widetilde{\mu}_i. \qquad (1.45)\end{aligned}$$

We can conclude that this potential is larger (in magnitude) for a given particle species within a reduced volume.

Density Dependent Degeneracy Factors

Using the definition for the reduced volume and degeneracy, we can define the effective degeneracy as a function of the volume, V as

$$g_i\widetilde{V} = g_i\left(V - \sum_i N_i V_i\right) = g_i\left(1 - \sum_i n_i V_i\right)V = \widetilde{g}_i V, \qquad (1.46)$$

with effective degeneracy factors

$$\widetilde{g}_i = g_i\left(1 - \sum_i n_i V_i\right), \qquad (1.47)$$

that depend on the particle densities n_i.

We define the grand canonical potential as

$$\widetilde{\Omega}(T,V,\widetilde{\mu}) = \sum_i \widetilde{\Omega}_i + W = T\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right) + m_i - \widetilde{\mu}_i, \tag{1.48}$$

where the individual particle contributions can be written as

$$\widetilde{\Omega}_i = -\frac{T\widetilde{g}_iV}{\sigma_i}\int\frac{d^3k}{(2\pi)^3}ln\left[1+\sigma_i\text{exp}\left(-\frac{\widetilde{U}_i-\widetilde{\mu}_i}{T}\right)\right], \tag{1.49}$$

with an additional contribution W. Here we introduce σ_i as we wish to generalize the particle contributions with consideration of different statistics - i.e. Fermi-Dirac and Bose-Einstein statistics in which $\sigma_i = 1$ for fermions and $\sigma_i = -1$ for bosons as discussed in (Carroll, 2007, p. 43), a boson is an integer-spin force-carrying particle, as opposed to a matter particle (fermion); and, unlike fermions, bosons can be accommodated to the same state without limit - e.g. photons, gluons, gravitons, weak bosons, and the Higgs boson. Also we define the single-particle energies as

$$\widetilde{U}_i(k) = \frac{k^2}{2m_i} + m_i + U_i. \tag{1.50}$$

Combining this with $\widetilde{\mu}_i$, we obtain

$$\begin{aligned}\widetilde{U}_i(k) - \widetilde{\mu}_i &= \frac{k^2}{2m_i} + m_i + U_i - \left[T \ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}} \right) + m_i + T V_i \sum_k \frac{N_k}{V - \sum\limits_j N_j V_j} \right], \\ &= \frac{k^2}{2m_i} + U_i - \left[T \ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}} \right) + T V_i \sum_k \frac{N_k}{V - \sum\limits_j N_j V_j} \right].\end{aligned}$$

Since $g_i \widetilde{V} = g_i \left(V - \sum_i N_i V_i \right) = g_i \left(1 - \sum_i n_i V_i \right) V = \widetilde{g}_i V$, we obtain

$$\begin{aligned}\widetilde{U}_i(k) - \widetilde{\mu}_i &= \frac{k^2}{2m_i} + U_i - T \ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}} \right) - T V_i \sum_i \frac{N_i}{g_j \widetilde{V}}, \\ &= \frac{k^2}{2m_i} + U_i - T \left[\ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}} \right) - V_i \sum_i \frac{N_i}{g_j \widetilde{V}} \right].\end{aligned}$$

That is

$$\begin{aligned}\frac{\widetilde{U}_i(k) - \widetilde{\mu}_i}{T} &= \frac{k^2}{2m_i T} + \frac{U_i}{T} - \ln\left(\frac{N_i {\lambda_i}^3}{g_i \widetilde{V}} \right) + V_i \sum_i \frac{N_i}{g_j \widetilde{V}}, \\ &= \frac{k^2}{2m_i T} + \frac{U_i}{T} + \ln\left(\frac{g_i \widetilde{V}}{N_i {\lambda_i}^3} \right) + V_i \sum_i \frac{N_i}{g_j \widetilde{V}}.\end{aligned}$$

Hence, we can calculate the particle number, N_i using

$$\begin{aligned}\frac{\partial}{\partial x}\ln\left[a\exp\left(\frac{x+y}{b}\right)+1\right] &= \frac{a\exp\left(\frac{x+y}{b}\right)}{\left(a\exp\left(\frac{x+y}{b}\right)+1\right)b} = \frac{a}{b}\frac{\exp\left(\frac{x+y}{b}\right)}{a\exp\left(\frac{x+y}{b}\right)+1},\\ &= \frac{a}{b}\frac{1}{a+\exp\left(\frac{-(x+y)}{b}\right)}.\end{aligned} \tag{1.51}$$

Since

$$\widetilde{\Omega}(T,V,\widetilde{\mu}) = T\ln\left(\frac{N_i{\lambda_i}^3}{g_i\widetilde{V}}\right)+m_i-\widetilde{\mu}_i,$$

then

$$-\frac{\partial\widetilde{\Omega}}{\partial\widetilde{\mu}_i}\bigg|_{T,V,\widetilde{\mu}_{j!=i}} = 1.$$

Hence

$$\begin{aligned}
N_i &\stackrel{!}{=} -\left.\frac{\partial\widetilde{\Omega}}{\partial\widetilde{\mu}_i}\right|_{T,V,\widetilde{\mu}_{j!=i}}, \\
&\stackrel{!}{=} +\frac{T\widetilde{g}_iV}{\sigma_i}\int\frac{d^3k}{(2\pi)^3}\frac{\sigma_i}{T}\frac{1}{\sigma_i+\exp\left(-\frac{-(\widetilde{U}_i-\widetilde{\mu}_i)}{T}\right)}-\frac{\partial W}{\partial\widetilde{\mu}_i}, \\
&= \frac{T\widetilde{g}_iV}{\sigma_i}\frac{\sigma_i}{T}\int\frac{d^3k}{(2\pi)^3}\frac{1}{\sigma_i+\exp\left(\frac{\widetilde{U}_i-\widetilde{\mu}_i}{T}\right)}-\frac{\partial W}{\partial\widetilde{\mu}_i}, \\
&= \widetilde{g}_iV\int\frac{d^3k}{(2\pi)^3}\frac{1}{\sigma_i+\exp\left(\frac{\widetilde{U}_i-\widetilde{\mu}_i}{T}\right)}-\frac{\partial W}{\partial\widetilde{\mu}_i}, \\
&= \widetilde{g}_iV\int\frac{d^3k}{(2\pi)^3}\left[\sigma_i+\exp\left(\frac{\widetilde{U}_i-\widetilde{\mu}_i}{T}\right)\right]^{-1}-\frac{\partial W}{\partial\widetilde{\mu}_i}, \\
&= \widetilde{g}_iV\int\frac{d^3k}{(2\pi)^3}\left[\sigma_i+\exp\left(\frac{k^2}{2m_iT}+\frac{U_i}{T}+\ln\left(\frac{g_i\widetilde{V}}{N_i\lambda_i{}^3}\right)+V_i\sum_i\frac{N_i}{g_j\widetilde{V}}\right)\right]^{-1} \\
&\quad -\frac{\partial W}{\partial\widetilde{\mu}_i}. \qquad (1.52)
\end{aligned}$$

Thus

$$\begin{aligned}
N_i &\stackrel{!}{=} -\left.\frac{\partial\widetilde{\Omega}}{\partial\widetilde{\mu}_i}\right|_{T,V,\widetilde{\mu}_{j!=i}}, \\
&\stackrel{!}{=} \widetilde{g}_iV\int\frac{d^3k}{(2\pi)^3}\left[\sigma_i+\exp\left(\frac{k^2}{2m_iT}+\frac{U_i}{T}+V_i\sum_i\frac{N_i}{g_j\widetilde{V}}+\left[\frac{1}{\ln\left(\frac{g_i\widetilde{V}}{N_i\lambda_i{}^3}\right)}\right]^{-1}\right)\right]^{-1} \\
&\quad -\frac{\partial W}{\partial\widetilde{\mu}_i},
\end{aligned}$$

which contains the "rearrangement" potentials U_i, defined by the relation between U_i *and* W as shown in the above relationship, in addition to the following

$$U_i = \sum_j \frac{\partial \widetilde{g}_j}{\partial N_i} \frac{\widetilde{\Omega}_i}{\widetilde{g}_i}. \tag{1.53}$$

Also noting that we can calculate $\partial W / \partial \widetilde{\mu}_i$,

$$\frac{\partial W}{\partial \widetilde{\mu}_i} = \widetilde{g}_i V \int \frac{d^3k}{(2\pi)^3} \left[\sigma_i + \exp\left(\frac{\widetilde{U}_i - \widetilde{\mu}_i}{T} \right) \right]^{-1} - 1.$$

Now,

$$g_i V = g_i \left(V - \sum_i N_i V_i \right) = g_i \left(1 - \sum_i n_i V_i \right) V = \widetilde{g}_i V, \tag{1.54}$$

$$\widetilde{g}_i = \frac{g_i}{V} \left(V - \sum_i N_i V_i \right) = g_i \left(1 - \sum_i n_i V_i \right), \tag{1.55}$$

Since $N_i = n_i V$

$$\frac{\partial \widetilde{g}_j}{\partial N_i} = \frac{1}{V} \frac{\partial \widetilde{g}_j}{\partial n_i} = -\frac{g_j \sum_i V_i}{V}. \tag{1.56}$$

Using this in U_i

$$\begin{aligned} U_i &= \sum_j \frac{\partial \widetilde{g}_j}{\partial N_i} \frac{\widetilde{\Omega}_i}{\widetilde{g}_i} = \frac{1}{V} \frac{\partial \widetilde{g}_j}{\partial n_i} \frac{\widetilde{\Omega}_i}{\widetilde{g}_i}, \\ &= \left(- \frac{g_j \sum_i V_i}{V} \right) \left(- \frac{TV}{\sigma_i} \int \frac{d^3k}{(2\pi)^3} ln \left[1 + \sigma_i \mathrm{exp} \left(- \frac{\widetilde{U}_i - \widetilde{\mu}_i}{T} \right) \right] \right), \\ &= \sum_i \frac{T g_j V_i}{\sigma_i} \int \frac{d^3k}{(2\pi)^3} ln \left[1 + \sigma_i \mathrm{exp} \left(- \frac{\widetilde{U}_i - \widetilde{\mu}_i}{T} \right) \right]. \end{aligned} \tag{1.57}$$

and using $N_i = n_i V$, we can now calculate the work,

$$\begin{aligned} W &= - \sum_i N_i U_i, \\ &= - \sum_i \frac{T g_i N_i V_i}{\sigma_i} \int \frac{d^3k}{(2\pi)^3} ln \left[1 + \sigma_i \mathrm{exp} \left(- \frac{\widetilde{U}_i - \widetilde{\mu}_i}{T} \right) \right], \\ &= - \sum_i \frac{T g_i n_i V_i V}{\sigma_i} \int \frac{d^3k}{(2\pi)^3} ln \left[1 + \sigma_i \mathrm{exp} \left(- \frac{\widetilde{U}_i - \widetilde{\mu}_i}{T} \right) \right]. \end{aligned} \tag{1.58}$$

Combining these results, we get

$$\frac{\partial \widetilde{g}_j}{\partial N_i} = \frac{1}{V} \frac{\partial \widetilde{g}_j}{\partial n_i} = - \frac{g_j \sum_i V_i}{V}, \tag{1.59}$$

and

$$\frac{N_i}{g_j} \times \left(- \frac{g_j \sum_i V_i}{V} \right) = - \frac{\sum_i N_i V_i}{V}. \tag{1.60}$$

Since, $N_i = n_i V$, one has

$$-\frac{\sum_i N_i V_i}{V} = -\frac{\sum_i n_i V_i V}{V} = -\sum_i n_i V_i. \tag{1.61}$$

Therefore,

$$W = -\sum_i N_i U_i = \sum_i \frac{T g_j n_i V V_i}{\sigma_i} \int \frac{d^3k}{(2\pi)^3} ln \left[1 + \sigma_i \text{exp} \left(-\frac{\widetilde{U}_i - \widetilde{\mu}_i}{T} \right) \right]. \tag{1.62}$$

We can combine all of these into a general equation

$$W = -\sum_i \sum_j \left(\frac{n_i V}{\widetilde{g}_j} \frac{\partial \widetilde{g}_j}{\partial N_i} \widetilde{\Omega}_j \right) = -\sum_{ij} \left(\delta_{ij} \frac{n_i V}{\widetilde{g}_j} \frac{\partial \widetilde{g}_j}{\partial N_i} \widetilde{\Omega}_j \right). \tag{1.63}$$

Thus, we have developed a prescription to include the density dependence of the degeneracy factors on the excluded volumes of the clusters.

Chapter 2

EQUATION OF STATE WITH EXCLUDED VOLUME

Introduction

The effects of the finite size of particles on the equation of state of a gas can be described with the help of the excluded-volume mechanism. It can also be used in order to simulate the suppression of a particular particle species, e.g. nuclei (clusters) in a mixture with nucleons, at high densities.

The excluded-volume mechanism can be formulated most simply by starting with the free energy $F(T, V, \{N_i\})$ of a classical ideal gas of particles i with single-particle numbers N_i in a volume V at temperature T. Instead of the total volume V of the system it is assumed that for a particle i only a reduced volume

$$V_i = V\Phi_i < V, \tag{2.1}$$

is available since part of the whole volume is occupied already by other particles. The functions $\Phi(n_i)$ depend on the single-particle densities $n_i = N_i/V$.

Applying a Legendre transformation

$$\Omega(T, V, \{\mu_i\}) = F - \sum_i \mu_i N_i = -pV, \tag{2.2}$$

with the chemical potentials (including rest masses m_i of the particles)

$$\mu_i = \left.\frac{\partial F}{\partial N_i}\right|_{T,V,\mu_{j\neq i}}, \tag{2.3}$$

where the grandcanonical potential Ω depends on the natural variables T, V, and the set $\{\mu_i\}$. It is better suited for generalizations of the model than the free energy F.

In the following, we use the usual system of units in nuclear physics with $\hbar = c = k_B = 1$. Thus these factors do not appear in the formulas explicitly but have to be considered in the conversion of quantities. Additionally, to more easily distinguish and compare the potentials derived from different physical constraints and arguments, we use labels of the form (id), (eff), (vi) , and (ex) as opposed to the use and absence of $\widetilde{X}$, (where X is the potential of interest), as in the previous chapter.

Classical Particles

Let us consider first classical particles with Maxwell-Boltzmann statistics and nonrelativistic kinematics without explicit interactions. In this case the grandcanonical potential is given by

$$\Omega = \sum_i \left(\Omega_i - N_i U_i\right), \tag{2.4}$$

with single-particle contributions

$$\Omega_i = -T g_i^{(\text{eff})} V \int \frac{d^3k}{(2\pi)^3} \, \exp\left[-\frac{E_i(k) - \mu_i}{T}\right], \tag{2.5}$$

and rearrangement potentials

$$U_i = \sum_j \frac{\partial g_j^{(\text{eff})}}{\partial N_i} \frac{\Omega_j}{g_j^{(\text{eff})}}, \tag{2.6}$$

that contain the density-dependent effective degeneracy factors

$$g_i^{(\text{eff})} = g_i \Phi_i, \tag{2.7}$$

and the energies (including rest masses m_i)

$$E_i(k) = \frac{k^2}{2m_i} + m_i + U_i. \tag{2.8}$$

of the particles. The usual degeneracy factors are denoted by g_i. They are constants. The rearrangement potentials U_i are essential in order to obtain a thermodynamically consistent model.

Ideal Gas

For the case of an ideal gas with pointlike particles, the functions Φ_i are just constants and equal to one such that the effective degeneracy factors $g_i^{(\mathrm{eff})}$ are identical to the usual degeneracy factors g_i of the particles and the rearrangement potentials U_i vanish. Then one finds explicitly as shown in (Typel, Röpkec, et al., 2010, p. 3)

$$\Omega^{(\mathrm{id})}(T, V, \{\mu_i^{(\mathrm{id})}\}) = -TV \sum_i \frac{g_i}{\lambda_i^3} \exp\left(\frac{\mu_i^{(\mathrm{id})} - m_i}{T}\right) = -p^{(\mathrm{id})} V, \tag{2.9}$$

and

$$N_i = - \left.\frac{\partial \Omega^{(\mathrm{id})}}{\partial \mu_i^{(\mathrm{id})}}\right|_{T,V,\mu_{j\neq i}} = V \frac{g_i}{\lambda_i^3} \exp\left(\frac{\mu_i^{(\mathrm{id})} - m_i}{T}\right), \tag{2.10}$$

with the thermal wavelengths

$$\lambda_i = \sqrt{\frac{2\pi}{m_i T}}, \tag{2.11}$$

such that the pressure of an ideal gas is given by

$$p^{(\mathrm{id})} = \frac{T}{V} \sum_i N_i \, , \tag{2.12}$$

i.e. the well-known relation for a mixture of classical ideal gases.

Classical Gas with Excluded Volume

Now we treat the case with explicit excluded-volume effects and assume that

$$\Phi_i(\{n_j\}) = 1 - \sum_j v_{ij} n_j , \tag{2.13}$$

with constant volumes v_{ij}. Sometimes these functions are defined as

$$\Phi_i(\{n_j\}) = 1 - \sum_j n_j v_j , \tag{2.14}$$

with volumes v_j of particles j such that the functions Φ_i are identical for all i. However, this leads to problems when the comparison to the virial equation of state is made, see below. Their relation to the volumes of the individual particles will be specified later.

One finds the single-particle contributions

$$\Omega_i^{(\mathrm{ex})} = -TV \frac{g_i^{(\mathrm{eff})}}{\lambda_i^3} \exp\left(\frac{\mu_i^{(\mathrm{ex})} - m_i - U_i}{T} \right) , \tag{2.15}$$

and the rearrangement potentials

$$U_i = \sum_j \frac{\partial \Phi_j}{\partial n_i} \frac{\Omega_j^{(\mathrm{ex})}}{V\Phi_j} = - \sum_j v_{ij} \frac{\Omega_j^{(\mathrm{ex})}}{V\Phi_j} . \tag{2.16}$$

All of these combined lead to the total excluded grandcanonical potential

$$\begin{aligned}
\Omega^{(\mathrm{ex})}(T,V,\{\mu_i\}) &= \sum_i \left(\Omega_i^{(\mathrm{ex})} + n_i \sum_j v_{ij} \frac{\Omega_j^{(\mathrm{ex})}}{\Phi_j} \right), \\
&= \sum_i \left(\sum_j \frac{\delta_{ij}\Phi_j}{\Phi_j} \Omega_i^{(\mathrm{ex})} + n_i \sum_j v_{ij} \frac{\Omega_j^{(\mathrm{ex})}}{\Phi_j} \right), \\
&= \sum_j \frac{\Phi_j}{\Phi_j} \Omega_j^{(\mathrm{ex})} + \sum_i n_i \sum_j v_{ij} \frac{\Omega_j^{(\mathrm{ex})}}{\Phi_j} \qquad (2.17) \\
&= \sum_j \frac{\Omega_j^{(\mathrm{ex})}}{\Phi_j}, \\
&= -T \sum_i \frac{g_i}{\lambda_i^3} V \ \exp\left(\frac{\mu_i^{(\mathrm{ex})} - m_i - U_i}{T} \right), \\
&= -p^{(\mathrm{ex})} V,
\end{aligned}$$

and the single-particle densities

$$n_i = -\frac{1}{V} \frac{\partial \Omega^{(\mathrm{ex})}}{\partial \mu_i^{(\mathrm{ex})}} = \frac{g_i^{(\mathrm{eff})}}{\lambda_i^3} \ \exp\left(\frac{\mu_i^{(\mathrm{ex})} - m_i - U_i}{T} \right) \ . \qquad (2.18)$$

Thus we find the relation

$$p^{(\mathrm{ex})} = T \sum_i \frac{n_i}{\Phi_i} \ . \qquad (2.19)$$

Since $\Phi_i < 1$, the pressure $p^{(\mathrm{ex})}$ with excluded-volume effects is larger than that of an ideal gas $p^{(\mathrm{id})}$ with the same particle number densities n_i.

Series Expansion

The grandcanonical potential $\Omega^{(\mathrm{ex})}$ can be expanded in powers of fugacities as in (Typel, Röpkec, et al., 2010, p. 3)

$$z_i = \exp\left(\frac{\mu_i^{(\mathrm{ex})} - m_i}{T}\right) \, , \tag{2.20}$$

by using the results for the rearrangement potentials U_i, and using a similar approach as in eq. (2.17). We find

$$\begin{aligned}
\Omega^{(\mathrm{ex})}(T, V, \{\mu_i\}) &= -T \sum_i \frac{g_i}{\lambda_i^3} V z_i \, \exp\left(-\frac{U_i}{T}\right) , \\
&= -T \sum_i \frac{g_i}{\lambda_i^3} V z_i \left[1 - \frac{U_i}{T} + \frac{1}{2}\left(\frac{U_i}{T}\right)^2 - \ldots\right] , \\
&\approx -T \sum_i \frac{g_i}{\lambda_i^3} V z_i \left(1 + \frac{1}{T} \sum_j v_{ij} \frac{\Omega_j^{(\mathrm{ex})}}{V \Phi_j} + \ldots\right) , \qquad (2.21) \\
&\approx -TV \sum_i \frac{g_i}{\lambda_i^3} z_i \left(1 - \sum_j v_{ij} \frac{g_j}{\lambda_j^3} z_j + \ldots\right) , \\
&= -TV \left(\sum_i \frac{g_i}{\lambda_i^3} z_i - \sum_{ij} v_{ij} \frac{g_i g_j}{\lambda_i^3 \lambda_j^3} z_i z_j + \ldots\right) ,
\end{aligned}$$

up to second order in the fugacities as also shown in Typel, Röpkec, et al. (2010).

Low-density Limit

So far we have considered the general formulation of the excluded-volume mechanism. However, the volumes v_{ij} are not fixed yet. In order to relate them to the volumes of the individual particles, the exact low-density limit of the equation of state can be used to define them.

Virial Expansion

At finite temperatures, the low-density limit is given by the virial equation of state. It is an expansion of the grandcanonical potential

$$\Omega^{(\mathrm{vi})}(T,V,\{\mu_i^{(\mathrm{vi})}\}) = -TV\left(\sum_i \frac{b_i}{\lambda_i^3} z_i + \sum_{ij} \frac{b_{ij}}{\lambda_i^{3/2}\lambda_j^{3/2}} z_i z_j + \dots\right), \qquad (2.22)$$

in powers of the fugacities

$$z_i = \exp\left(\frac{\mu_i^{(\mathrm{vi})} - m_i}{T}\right), \qquad (2.23)$$

with dimensionless virial coefficients b_i, b_{ij}, ... The expansion is valid only for $z_i \ll 1$ or $n_i\lambda_i^3 \ll 1$. The first virial coefficients $b_i = g_i$ are just the standard degeneracy factors.

Classical Mechanics

The second virial coefficients in classical mechanics are given by

$$b_{ij}^{(\mathrm{cl})}(T) = \frac{1+\delta_{ij}}{2}\frac{g_i g_j}{\lambda_i^{3/2}\lambda_j^{3/2}}\int d^3r\left[\exp\left(-\frac{V_{ij}}{T}\right)-1\right], \tag{2.24}$$

depending on the potential V_{ij} between the particles i and j. For incompressible spherical particles with radii R_i and volumes $V_i = 4\pi R_i^3/3$ it is given by the hard-sphere potential

$$V_{ij}(r) = \begin{cases} \infty & \text{if} \quad r \leq R_{ij}, \\ 0 & \text{if} \quad r > R_{ij}, \end{cases} \tag{2.25}$$

with the sum of the radii $R_{ij} = R_i + R_j$. Then we have

$$b_{ij}^{(\mathrm{cl})}(T) = \frac{1+\delta_{ij}}{2}\frac{g_i g_j}{\lambda_i^{3/2}\lambda_j^{3/2}}4\pi\int_0^{R_{ij}} dr\, r^2\,[-1] = -\frac{1+\delta_{ij}}{2}\frac{g_i g_j}{\lambda_i^{3/2}\lambda_j^{3/2}}\frac{4\pi}{3}R_{ij}^3\,. \tag{2.26}$$

Comparing with the result for the series expansion of $\Omega^{(\mathrm{ex})}$ we can identify

$$v_{ij} = \frac{1+\delta_{ij}}{2}\frac{4\pi}{3}R_{ij}^3, \tag{2.27}$$

if we set $\mu_i^{(\mathrm{ex})} = \mu^{(\mathrm{cl})}$. In particular we find

$$v_{ii} = \frac{4\pi}{3}(2R_i)^3 = 8V_i, \tag{2.28}$$

because the centers of two equal particles cannot become closer than twice their radius.

Quantum Mechanical Effects

The classical expression for the second virial coefficient does not take into account quantum effects. Using the formalism described in both Uhlenbeck & Beth (1936) and Beth & Uhlenbeck (1937), the quantum-mechanical second virial coefficient (without additional quantum-statistical corrections for Fermions or Bosons) is given by

$$b_{ij}^{(\mathrm{qu})}(T) = \frac{1+\delta_{ij}}{2}\frac{\lambda_i^{3/2}\lambda_j^{3/2}}{\lambda_{ij}^3}\int dE\ \exp\left(-\frac{E}{T}\right) D_{ij}(E), \tag{2.29}$$

with

$$\lambda_{ij} = \sqrt{\frac{2\pi}{(m_i+m_j)T}}, \tag{2.30}$$

and the kinetic energy of the relative motion

$$E = \frac{k^2}{2\mu_{ij}}, \tag{2.31}$$

that contains the reduced mass

$$\mu_{ij} = \frac{m_i m_j}{m_i+m_j}\ . \tag{2.32}$$

From these we can then determine the “level density” difference as shown in Typel, Röpkec, et al. (2010)

$$D_{ij}(E) = \sum_k g_k^{(ij)} \delta(E - E_k^{(ij)}) + \sum_l \frac{g_l^{(ij)}}{\pi} \frac{d\delta_l^{(ij)}}{dE}, \tag{2.33}$$

with

$$g_l^{(ij)} = (2l + 1) g_i g_j, \tag{2.34}$$

which contains contributions from two-particle bound states k and scattering states l in partial-wave expansion (neglecting spin-dependent potentials). Notably, we don’t have bound states for the hard-sphere potential but only scattering states. Hence, we need the scattering phase shifts $\delta_l^{(ij)}$ in all partial waves l as a function of the relative momentum k. Using that, we can then calculate the second virial coefficients

$$b_{ij}^{(\mathrm{qu})}(T) = \sum_l b_{ij}^{(l)}(T), \tag{2.35}$$

with

$$b_{ij}^{(l)}(T) = \frac{1 + \delta_{ij}}{2} \frac{(2l + 1) g_i g_j}{\pi} \frac{\lambda_i^{3/2} \lambda_j^{3/2}}{\lambda_{ij}^3} \int_0^\infty dk \, \exp\left(-\frac{k^2}{2\mu_{ij} T}\right) \frac{d\delta_l^{(ij)}}{dk}. \tag{2.36}$$

To include quantum effects we need to solve the time-independent Schrödinger equation

$$H_{ij}\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{2.37}$$

with the Hamiltonian as

$$H_{ij} = \frac{p^2}{2\mu_{ij}} + V_{ij}, \tag{2.38}$$

to obtain the scattering wave function ψ for the relative motion at energy $E = k^2/(2\mu_{ij})$ which can be written as

$$\psi_{ij}(\mathbf{r}) = \frac{4\pi}{kr}\sum_{lm} i^l u_l^{(ij)}(r) Y_{lm}(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{r}}), \tag{2.39}$$

with spherical harmonics Y_{lm} that depend on the direction of the coordinate and momentum vectors $\mathbf{r}$ and $\mathbf{k}$, respectively. The radial wave functions $u_l^{(ij)}(r)$ have to fulfill the boundary conditions in each partial wave l. In case of the hard-sphere potential, the radial wave functions for $r \geq R_{ij}$ have the form

$$u_l^{(ij)}(r) = \frac{1 + S_l^{(ij)}}{2}\left[F_l(kr) + K_l^{(ij)} G_l(kr)\right], \tag{2.40}$$

with the S-matrix elements are given in terms of the phase shifts δ by means of

$$S_l^{(ij)} = \exp\left(2i\delta_l^{(ij)}\right), \tag{2.41}$$

and the K-matrix elements are

$$K_l^{(ij)} = \frac{1}{i}\frac{S_l^{(ij)} - 1}{S_l^{(ij)} + 1} = \tan\delta_l^{(ij)}. \tag{2.42}$$

Of these, the regular and irregular scattering wave functions can be expressed with the help of spherical Bessel functions

$$F_l(z) = zj_l(z), \tag{2.43}$$

$$G_l(z) = -zy_l(z), \tag{2.44}$$

with the asymptotics

$$F_l(z) \rightarrow \sin\left(z - l\frac{\pi}{2}\right), \tag{2.45}$$

$$G_l(z) \rightarrow \cos\left(z - l\frac{\pi}{2}\right), \tag{2.46}$$

for $z \rightarrow \infty$. On the other hand, we have

$$F_l(z) \rightarrow \frac{z^l}{(2l+1)!!}, \tag{2.47}$$

$$G_l(z) \rightarrow \frac{(2l-1)!!}{z^{l+1}}, \tag{2.48}$$

for $z \rightarrow 0$. For $r \leq R_{ij}$ the radial wave function should vanish. This condition

$$u_l(R_{ij}) = 0, \tag{2.49}$$

leads to

$$\tan \delta_l^{(ij)} = -\frac{F_l(kR_{ij})}{G_l(kR_{ij})} = \frac{j_l(kR_{ij})}{y_l(kR_{ij})} \, . \tag{2.50}$$

Hence, we can calculate $\delta_l^{(ij)}$ for all k and l. For $l = 0$ we explicitly have

$$\tan \delta_0^{(ij)} = -\frac{\sin(kR_{ij})}{\cos(kR_{ij})}, \tag{2.51}$$

or

$$\delta_0^{(ij)} = -kR_{ij} \, . \tag{2.52}$$

With help of the equations developed so far for the statistics and thermodynamics of particles with finite size, we can pave the road to understand the effects of excluded volume mechanism on the equation of state for a gas of nucleons and nuclei. Our analysis is not complete, but we show the effects in a few numerical exercises in the next chapter.

Chapter 3

NUMERICAL STUDIES

In order to see the differences between the various equations of states and their approximations, numerical calculations have to be performed. We will study different systems in the following.

Single species with finite volume

As a first application we consider a single particle species i. In order to have realistic numbers we choose neutrons ($i = n$) as an example with rest mass $m_n = 939.565$ MeV/c^2 and degeneracy factor $g_n = 2$. We set the radius to $R_n = 0.5$ fm, $R_{nn} = 1.0$ fm and the volume

$$v_{nn} = \frac{1}{2}\frac{4\pi}{3}R_{nn}^3 \approx 2.094 \text{ fm}^3 \, . \tag{3.1}$$

Then the function

$$\Phi_n = 1 - v_{nn}n_n \, , \tag{3.2}$$

which appears in the effective degeneracy factor

$$g_n^{(\text{eff})} = g_n\Phi_n \, , \tag{3.3}$$

with the neutron density n_n becomes zero at the maximum density

$$n_n^{(\max)} = \frac{1}{v_{nn}} \approx 0.4775 \text{ fm}^{-3} \, . \tag{3.4}$$

Thus the equation of state with the excluded volume can be calculated only for neutron densities $0 < n_n < n_n^{(\max)}$.

Virial coefficients with excluded volume

Recalling the virialized coefficients $b_{ij}^{(l)}$ are functions of the partial waves, then as a first step in calculating the neutron-neutron scattering phases shifts we calculate from eq. (2.50)

$$\begin{aligned} \tan \delta_l^{(ij)} &= -\frac{F_l(kR_{ij})}{G_l(kR_{ij})} = \frac{j_l(kR_{ij})}{y_l(kR_{ij})}, \\ \delta_l^{(ij)} &= \arctan\left[\frac{j_l(kR_{ij})}{y_l(kR_{ij})}\right] \end{aligned} \tag{3.5}$$

for the specific case where $i = j = n$ is given by

$$\delta_l^{(nn)} = \arctan\left[\frac{j_l(kR_{nn})}{y_l(kR_{nn})}\right] \tag{3.6}$$

as a function of k for partial waves $l = 0, 1, 2, \ldots$ This is shown in Figure (1), for the interval $[0\ \mathrm{MeV/c}, 200\ \mathrm{MeV/c}]$.

Then, using (3.6), we can also find the derivatives, $d\delta_l^{(nn)}/dk$ for the same interval $[0\ \mathrm{MeV/c}, 200\ \mathrm{MeV/c}]$ as shown in Figure (2). All of this information can then be used to find the partial contributions

$$b_{nn}^{(l)}(T) = \frac{(2l+1)g_n^2}{\pi}\frac{\lambda_n^3}{\lambda_{nn}^3}\int_0^\infty dk\ \exp\left(-\frac{k^2}{2\mu_{nn}T}\right)\frac{d\delta_l^{(ij)}}{dk} \tag{3.7}$$

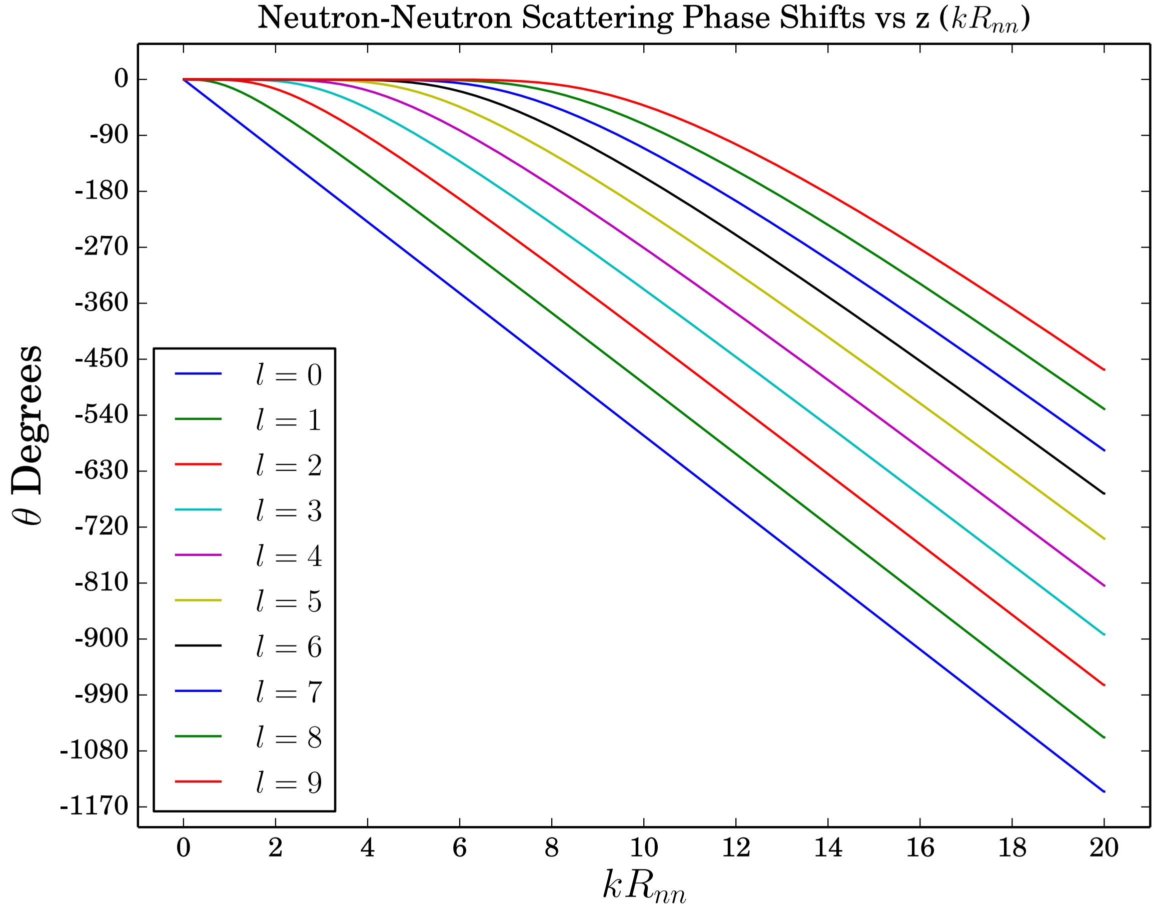

Figure 1. Neutron-neutron scattering phase-shifts (θ degrees) vs z (kR_{nn}) within the limit $[0, 20]$.

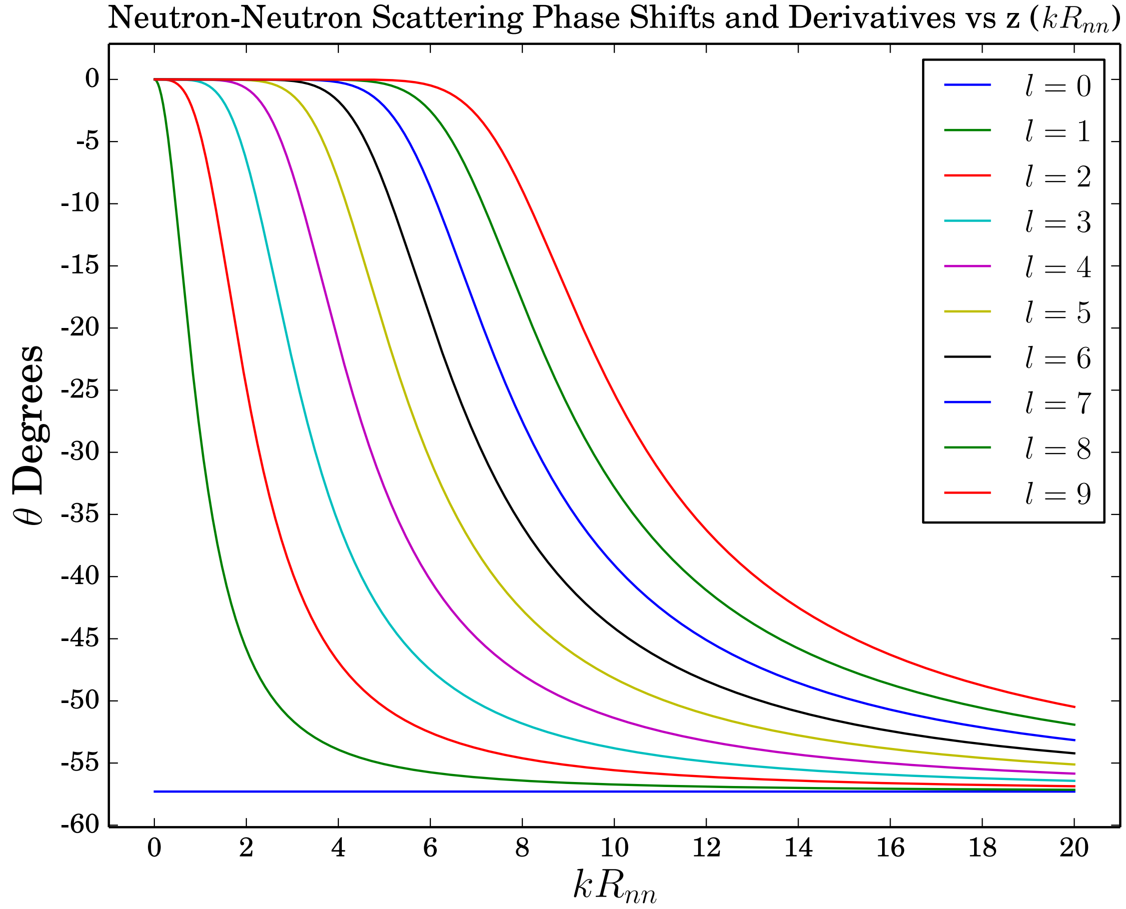

Figure 2. Neutron-neutron phase-shift derivatives vs $z = kR_{nn}\ \forall\ z \in [0, 20]$.

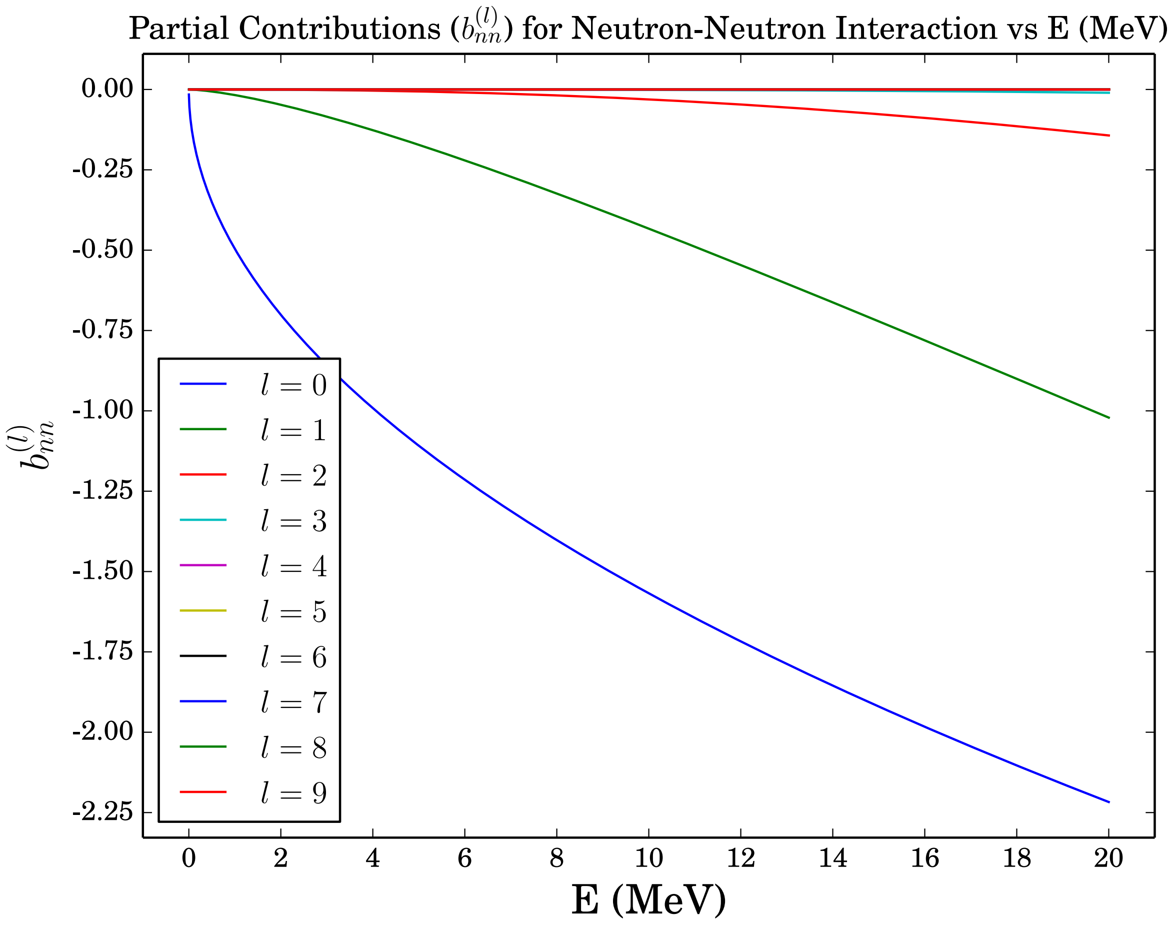

Figure 3. Partial contributions for neutron-neutron interaction vs energy (MeV) $\forall \;\; E \in [0MeV, 20MeV]$.

to the second virial coefficient $b_{nn}(T)$ as a function of T inside the interval $[0\ \mathrm{MeV}, 20\ \mathrm{MeV}]$ for $l = 0, 1, 2, \ldots$ shown in Figure (3).

Using (3.7), we can then calculate the total second virial coefficient, which is given by as an infinite sum

$$b_{nn}^{(\mathrm{qu})}(T) = \sum_{l=0}^{\infty} b_{nn}^{(l)}(T)\ . \tag{3.8}$$

However, while the total second virial coefficient (in the quantum mechanics case) can be analytically calculated as an infinite sum (for l > 0), the function converges relatively quickly and only 6 l-values are required to achieve convergence (within 3.4 parts per million), as shown in Figure (4).

Similarly, we can calculate the classical second virial coefficient as a function of the temperature, T which is given by the following equation (and as illustrated as shown in Figure (5))

$$b_{nn}^{(\mathrm{cl})}(T) = -\frac{g_n^2}{\lambda_n^3}\frac{4\pi}{3}R_{nn}^3 \tag{3.9}$$

Finally, we can compare the classical second virial coefficient with the quantum mechanical version both as functions of T, and we obtain Figure (6) which definitely shows a disparity between both. This makes sense since a classical billiard ball treatment doesn't take into consideration quantum effects at short distances.

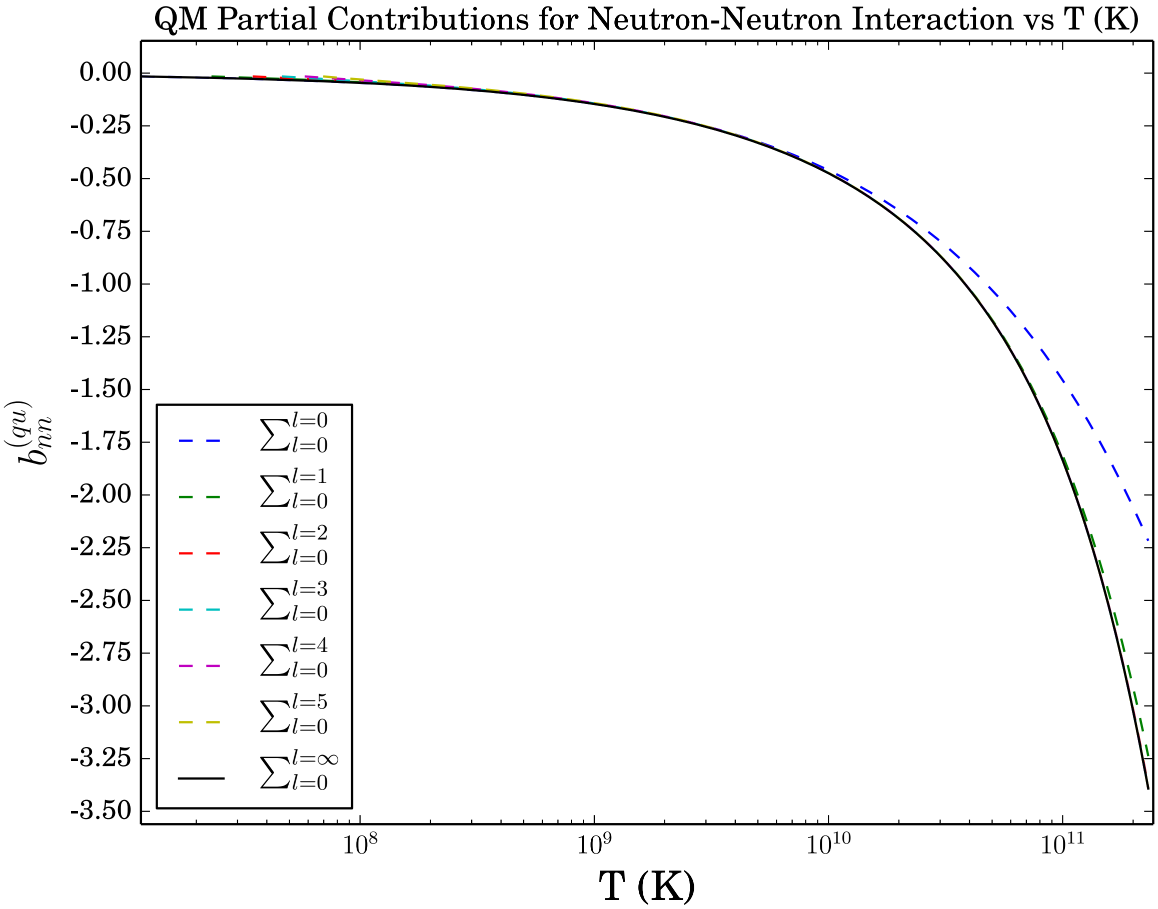

Figure 4. Quantum mechanical partial contributions for neutron-neutron interaction vs temperature (K).

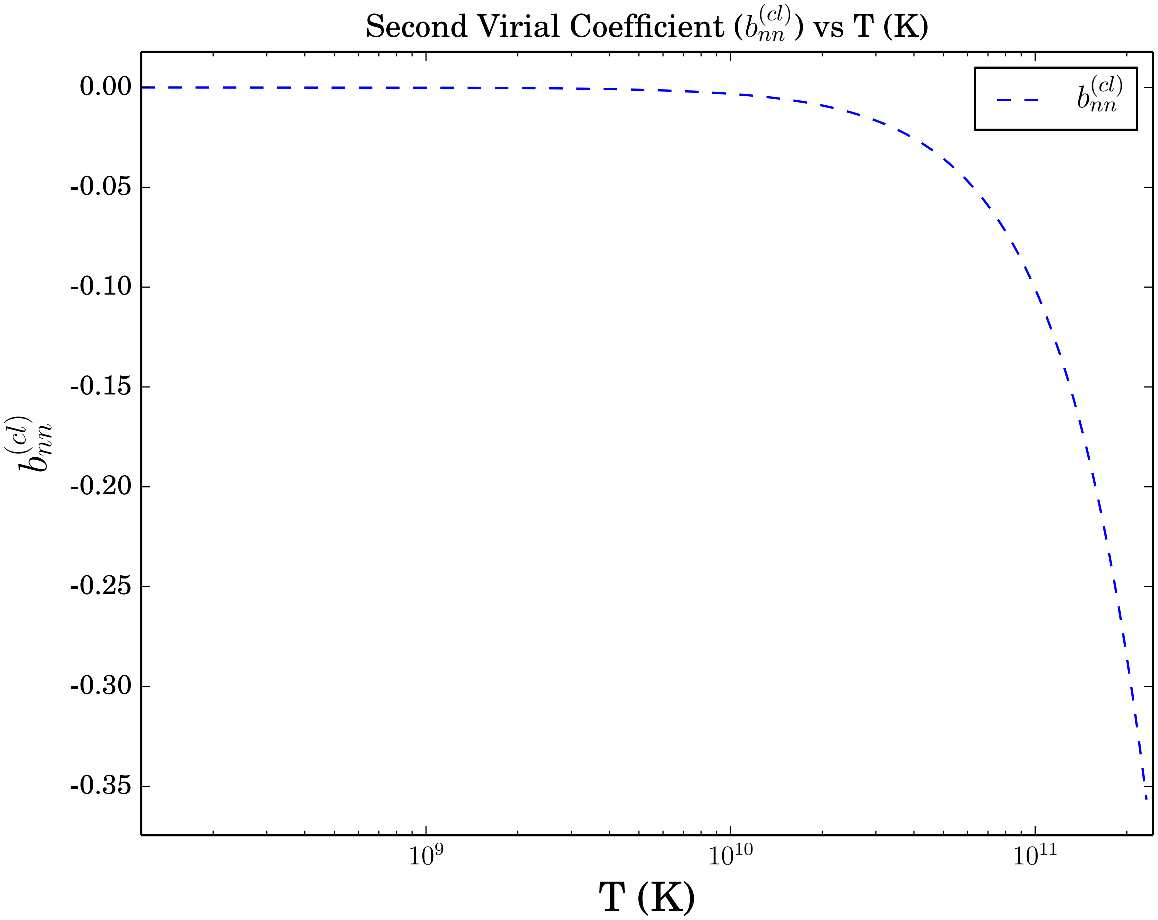

Figure 5. Semi-log plot of classical $b_{nn}^{(cl)}$ vs temperature (K).

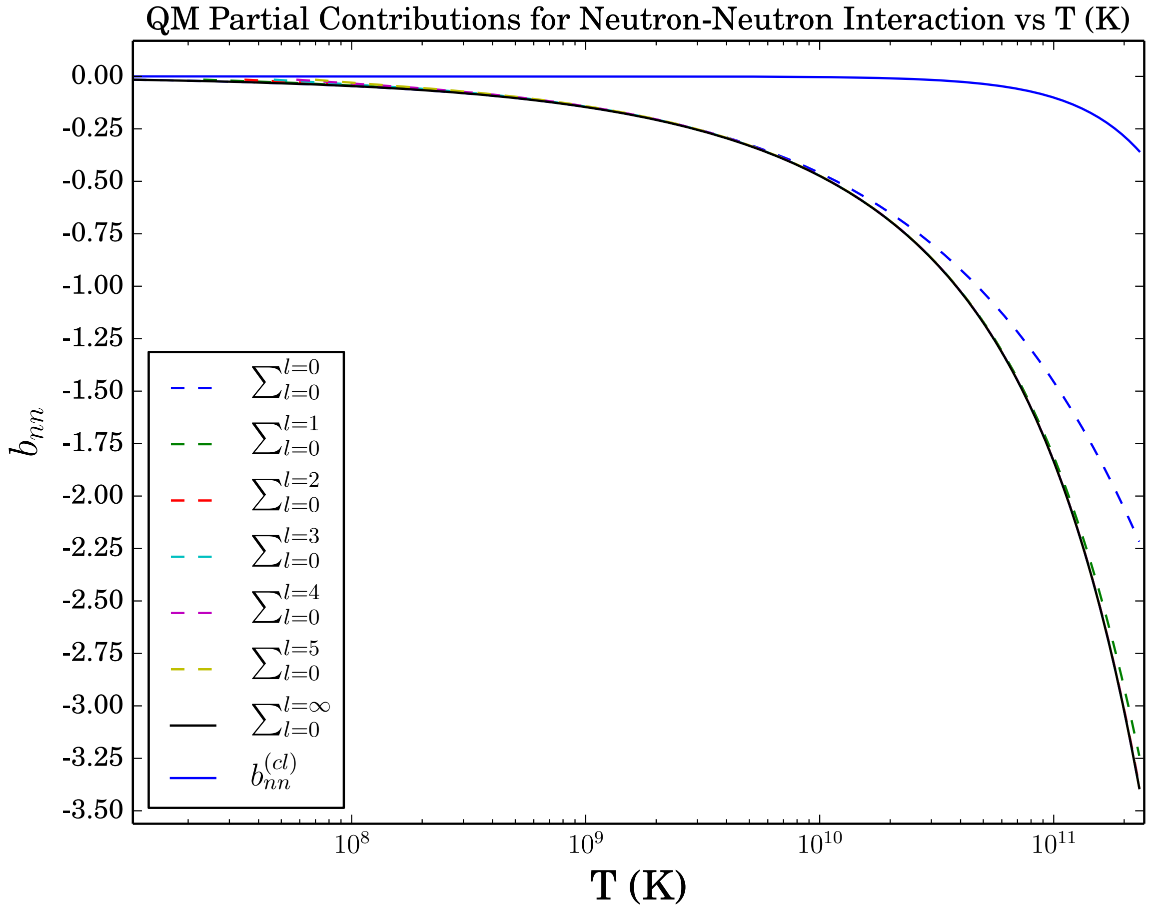

Figure 6. Semi-log plot comparing classical and quantum mechanical partial contributions ($b_{nn}^{(qu)}(T)$) for Neutron-Neutron Interaction vs Temperature (K).

To examine this even further, we then calculate the function, called the S-Function

$$S(z) = -\frac{1}{z^2} \sum_{l=0} \frac{2l+1}{[j_l(z)^2] + [j_l(z)^2]}. \tag{3.10}$$

Which, for the interval, $z \in [0, 20]$ is shown in Figure (7). Then, defining an approximation to this function (i.e. a fitting function) as

$$\widetilde{S}(z) = -1 - \frac{3}{2}z - \frac{2}{3}z^2. \tag{3.11}$$

Next, after comparing both of these together in Figure (9) we observe that $\widetilde{S}$ is a good (and fast) approximation to the general S-function which involves spherical Bessel functions.

Finally, we can compare all three second virial coefficients $b_{nn}^{(cl)}(T)$, $b_{nn}^{(qu)}(T)$, $\widetilde{b}_{nn}^{(qu)}(T)$ as shown in Figure (10) and Figure (11) which illustrate that the $b_{nn}^{(qu)}(T)$, $\widetilde{b}_{nn}^{(qu)}(T)$ coefficients deviate from the classical case.

Virial Equation of State

With the known second virial coefficients $b_{nn}^{(\mathrm{qu})}(T)$ and $b_{nn}^{(\mathrm{cl})}(T)$ we can calculate the pressure

$$p^{(\mathrm{vi,qu})} = -\frac{\Omega^{(\mathrm{vi,qu})}(T, V, \mu_n^{(\mathrm{vi,qu})})}{V} = \frac{T}{\lambda_n^3}\left[g_n z_n^{(\mathrm{vi,qm})} + b_{nn}^{(\mathrm{qu})}\left(z_n^{(\mathrm{vi,qm})}\right)^2\right] \tag{3.12}$$

and

$$p^{(\mathrm{vi,cl})} = -\frac{\Omega^{(\mathrm{vi,cl})}(T, V, \mu_n^{(\mathrm{vi,cl})})}{V} = \frac{T}{\lambda_n^3}\left[g_n z_n^{(\mathrm{vi,cl})} + b_{nn}^{(\mathrm{cl})}\left(z_n^{(\mathrm{vi,cl})}\right)^2\right] \tag{3.13}$$

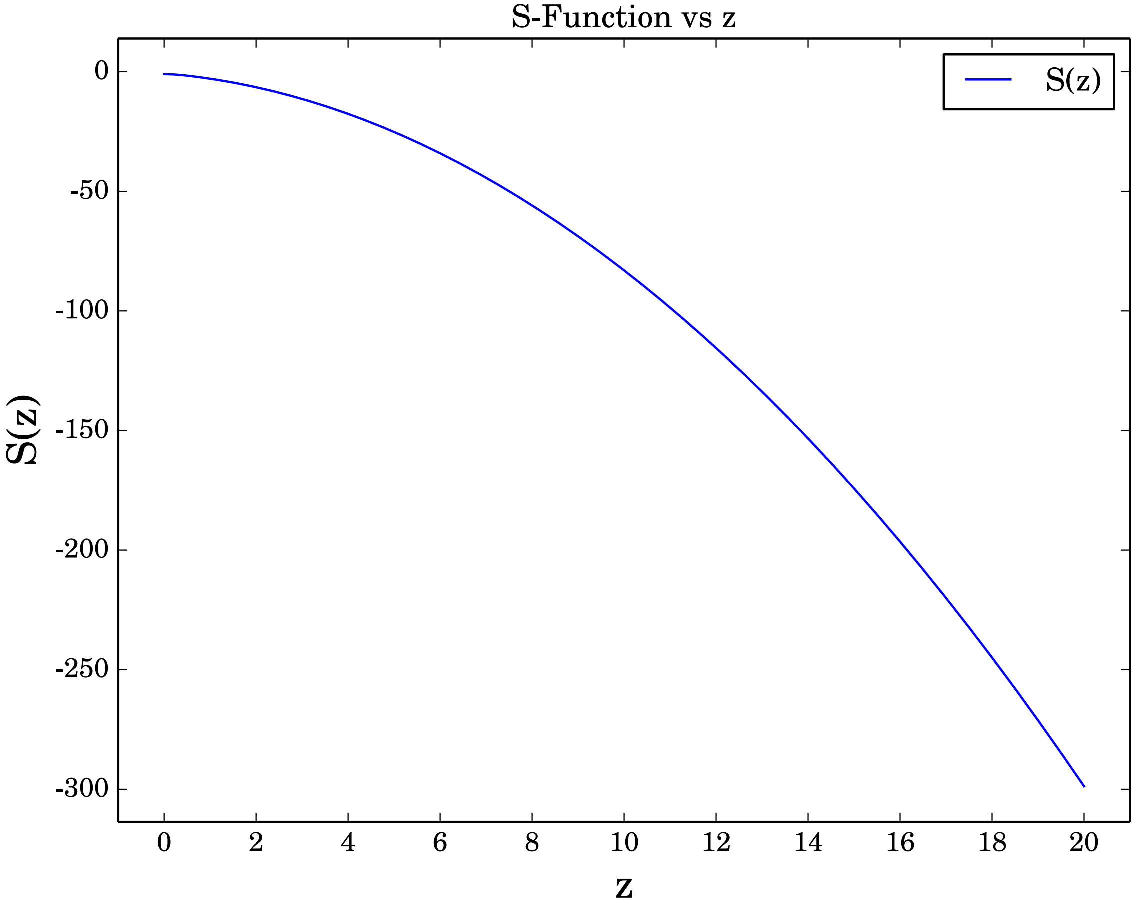

Figure 7. The second virial coefficient S-Function vs $z = kR_{nn}\ \forall\ z \in [0, 20]$.

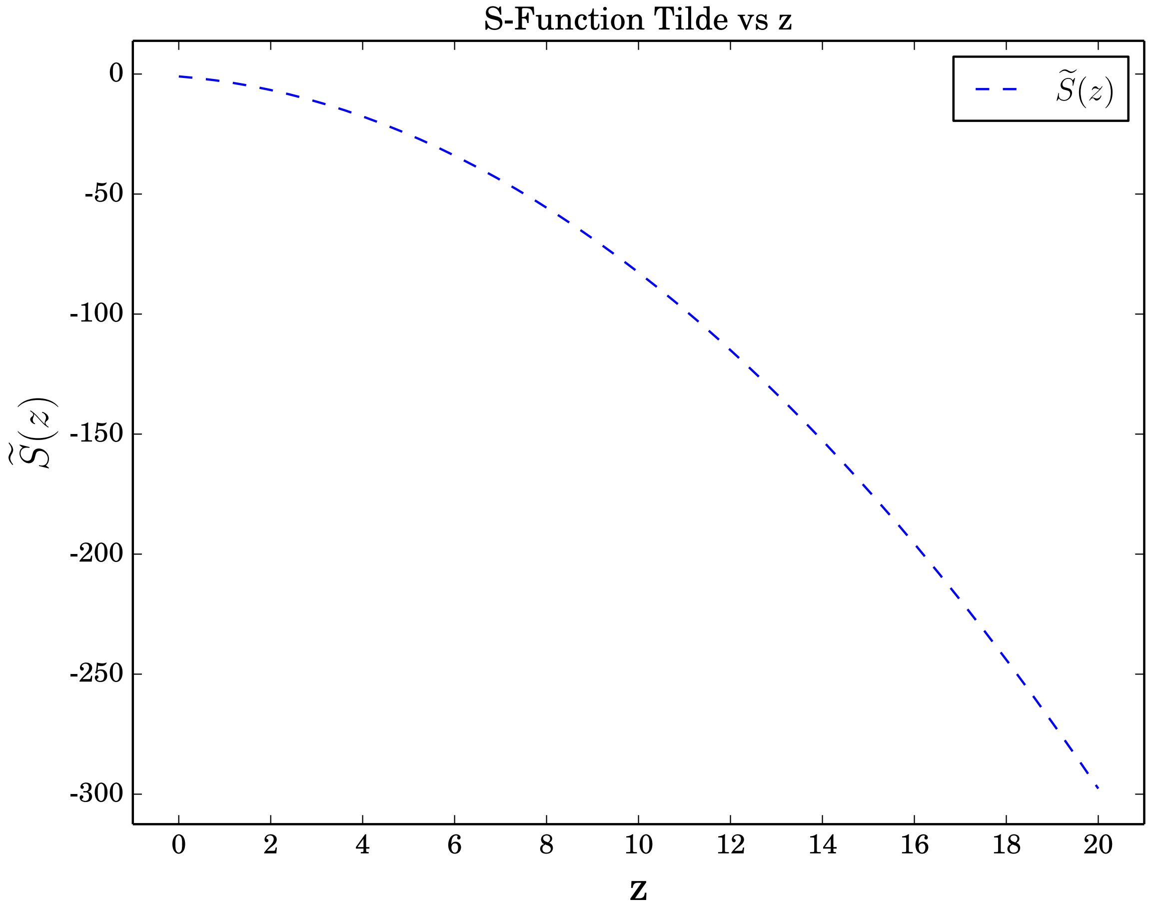

Figure 8. The second virial coefficient S-Function tilde vs $z = kR_{nn}$ $\forall$ $z \in [0, 20]$.

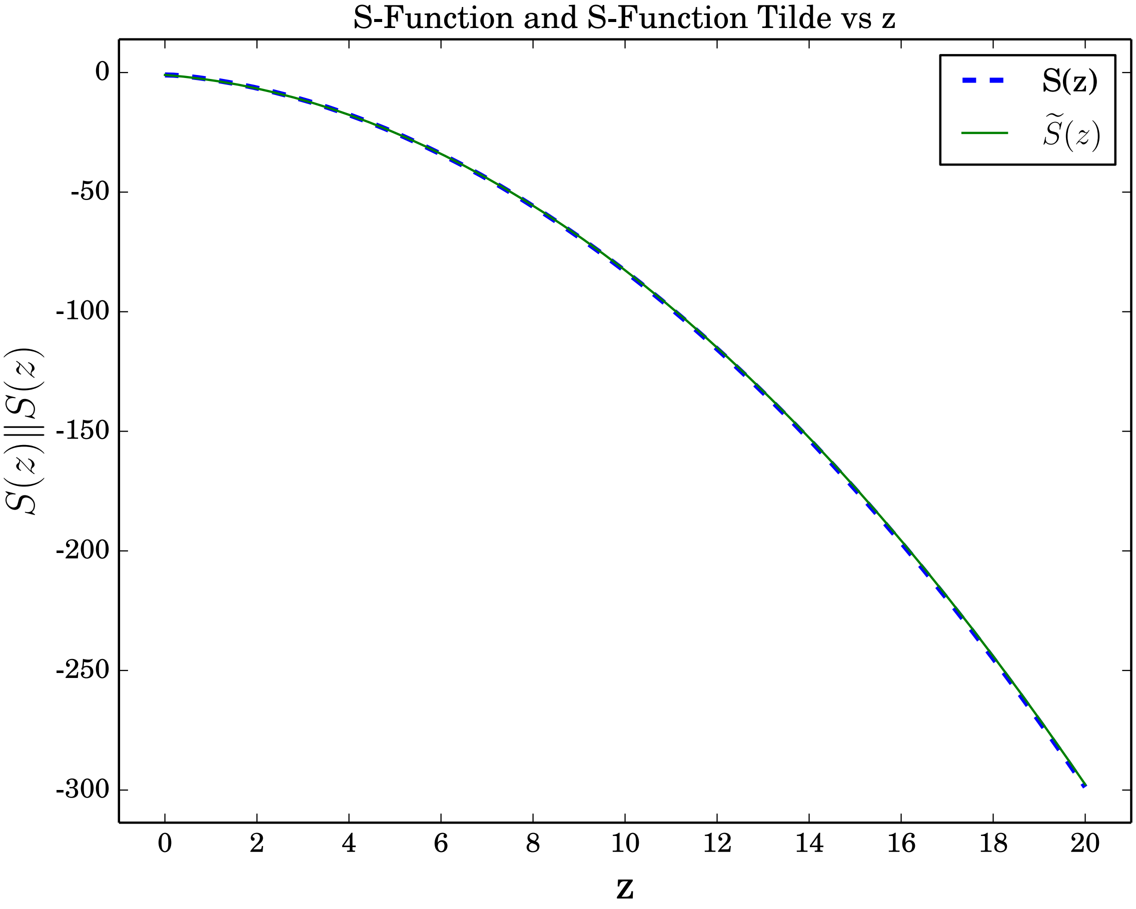

Figure 9. Comparison of the second virial coefficient S-Function, and S-Function tilde vs $z = kR_{nn} \ \forall \ z \in [0, 20]$.

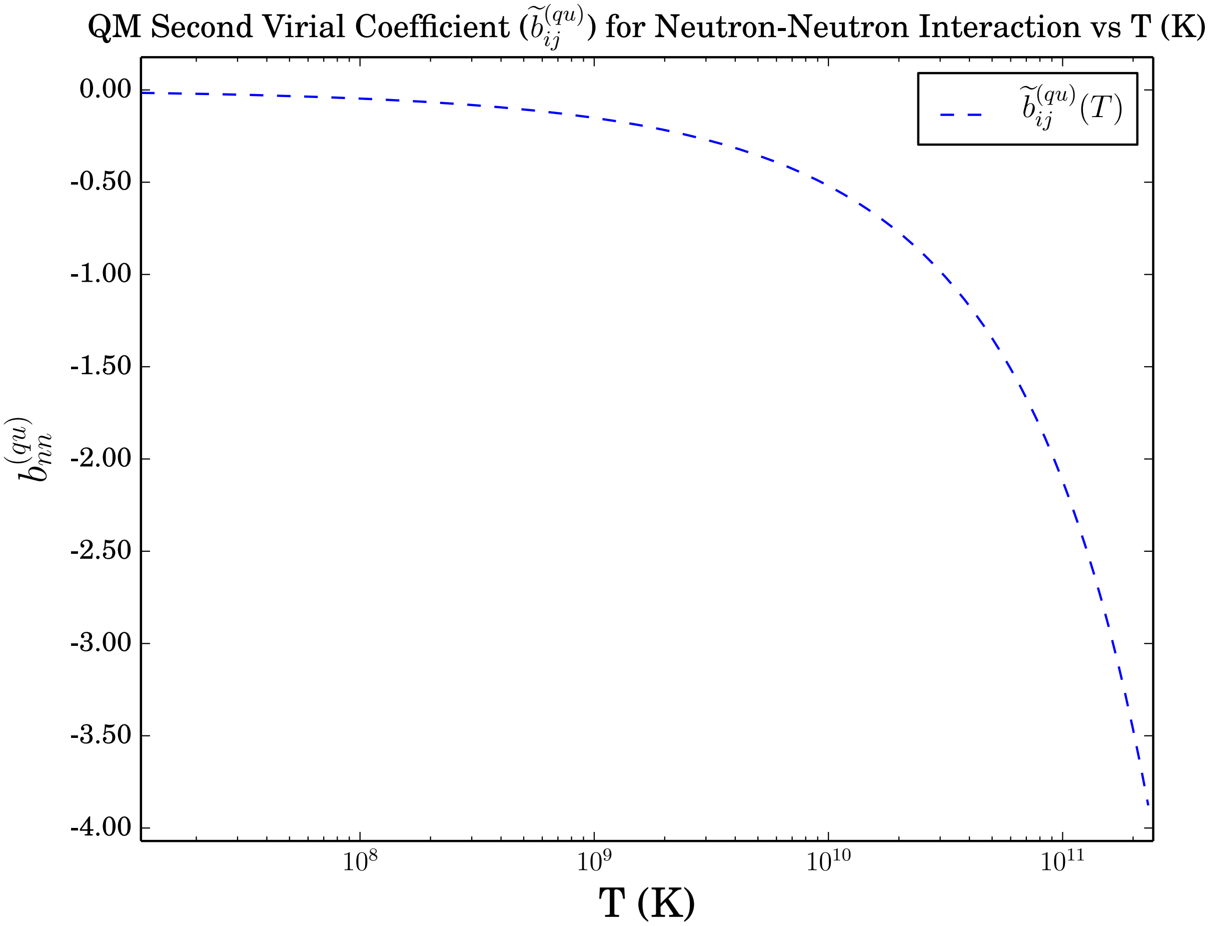

Figure 10. Semi-log plot of the QM second virial coefficient tilde $\widetilde{b}_{nn}^{(qu)}$ for neutron-neutron interaction vs temperature (T).

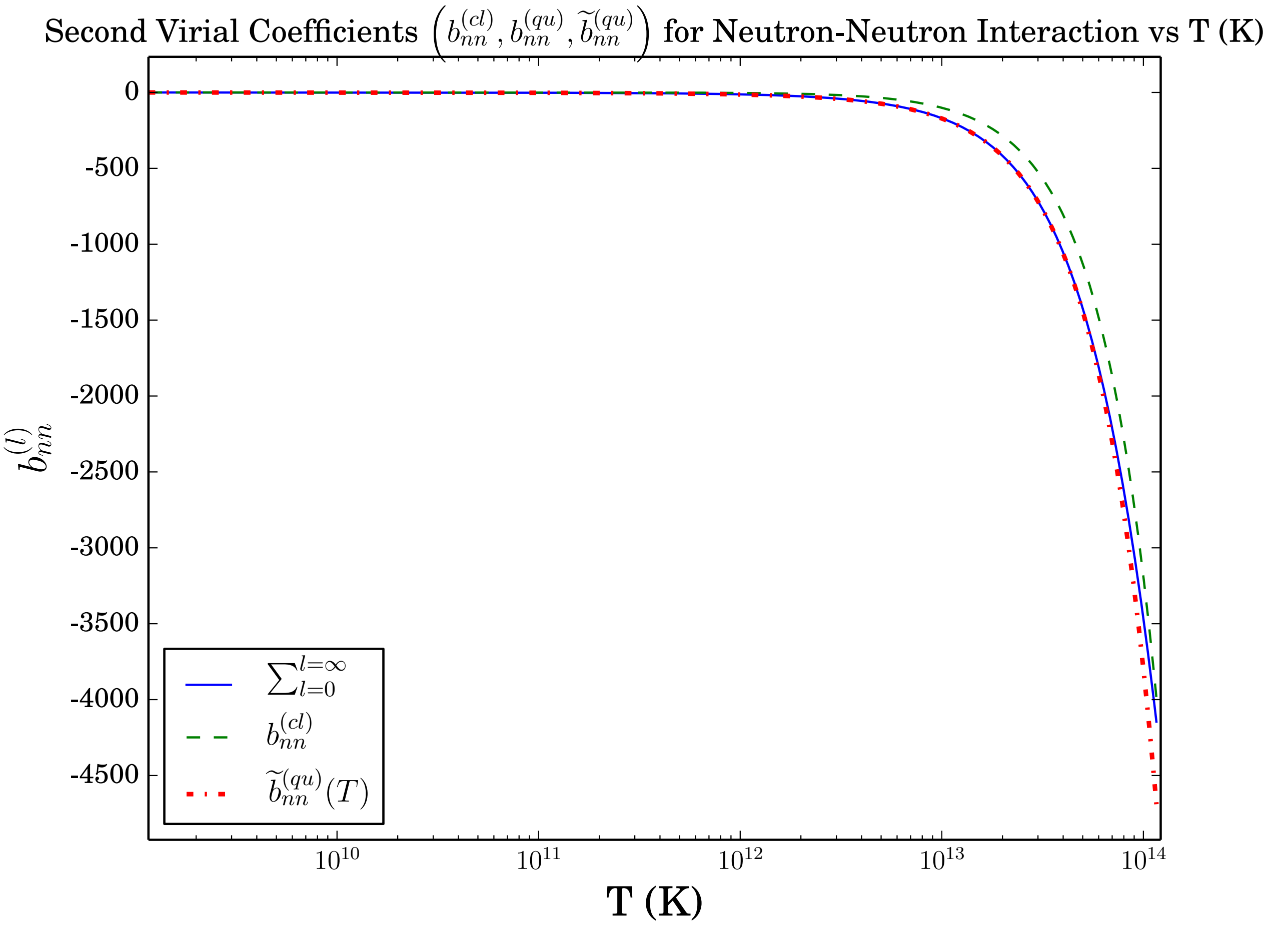

Figure 11. Semi-log plot of the second virial coefficients $\left(b_{nn}^{(cl)}, b_{nn}^{(qu)}, \widetilde{b}_{nn}^{(qu)}\right)$ for neutron-neutron interaction vs temperature (K).

in the two approximations for the virial equation of state. In order to obtain the fugacities

$$z_n^{(\mathrm{vi,qm})} = \exp\left(\frac{\mu_n^{(\mathrm{vi,qm})} - m_n}{T}\right) \tag{3.14}$$

and

$$z_n^{(\mathrm{vi,cl})} = \exp\left(\frac{\mu_n^{(\mathrm{vi,cl})} - m_n}{T}\right) \tag{3.15}$$

we consider the neutron densities

$$n_n = \left.\frac{\partial p^{(\mathrm{vi,qu})}}{\partial \mu_n}\right|_T = \frac{1}{\lambda_n^3}\left[g_n z_n^{(\mathrm{vi,qm})} + 2b_{nn}^{(\mathrm{qu})}\left(z_n^{(\mathrm{vi,qm})}\right)^2\right] \tag{3.16}$$

and

$$n_n = \left.\frac{\partial p^{(\mathrm{vi,cl})}}{\partial \mu_n}\right|_T = \frac{1}{\lambda_n^3}\left[g_n z_n^{(\mathrm{vi,cl})} + 2b_{nn}^{(\mathrm{cl})}\left(z_n^{(\mathrm{vi,cl})}\right)^2\right] . \tag{3.17}$$

Using these two (quadratic) equations, we can find the fugacities for given temperature T and density n_n. In a second step, the pressure can be calculated.

Mixture of Nucleons and Deuterons

To observe the effect of volume-exclusion, we consider a classical mixture of neutrons, protons and deuterons in chemical and thermal equilibrium.

From these considerations we can calculate the particle number densities from

$$n_i = \frac{g_i}{\lambda_i^3}\exp\left(\frac{\mu_i^{(id)} - m_i}{T}\right) \tag{3.18}$$

where we use the following constraints

Table 1

Particle masses and degeneracies.

Particle	Mass (MeV/c^2)	Degeneracy
p	$m_p = 939.565$	$g_p = 2$
n	$m_n = 938.272$	$g_n = 2$
d	$m_d = 1875.612$	$g_d = 3$

and where the mass of Deuteron is calculated as: $m_d = m_n + m_p - B_d = 939.565 MeV/c^2 + 938.272 MeV/c^2 - 2.2225 MeV/c^2 = 1875.612 MeV/c^2$, ($B_d$ is the binding energy of the Deuteron nucleus ($2.2225 MeV/c^2$)).

As there are two independent densities, we can call this the total neutron number density as shown in (Typel, Röpke, et al., 2010, p. 3)

$$n_n^{(tot)} = n_n + n_d. \tag{3.19}$$

Similarly, for the proton number density (Typel, Röpke, et al., 2010, p. 3)

$$n_p^{(tot)} = n_p + n_d. \tag{3.20}$$

However, it is more convenient to introduce the total baryon number density n_B, which is a sum of the two

$$n_B = n_n^{(tot)} + n_p^{(tot)} = n_n + n_p + 2n_d. \tag{3.21}$$

Next, we also consider the iso-spin asymmetry which is defined as

$$\delta = \frac{n_n^{(tot)} - n_p^{(tot)}}{n_B} = \frac{n_n - n_p}{n_B} \tag{3.22}$$

However, while the total neutron and proton number densities are independent, the individual number densities of the neutrons, protons and deuterons are not - as they are constrained by the chemical equilibrium such that

$$\mu_n + \mu_p = \mu_d. \tag{3.23}$$

Point Particles ($R_i = 0$ (i = n, p, d))

To further understand this, we first consider a mixture of point particles of neutrons, protons and deuterons ($i = n, p, d$) such that $R_n = R_p = R_d = 0$ fm, and with $\delta = 0$ as shown in Figures (12), (13), and (14) for neutrons, protons and deuterons respectively.

From Figures (12), (13), and (14) we can assert that the deuteron mass fraction decreases with rising temperature, and increases slowly with increasing temperature and baryon density. The opposite effect is observed with the symmetric mixture of protons and neutrons, for increasing temperature and baryon density.

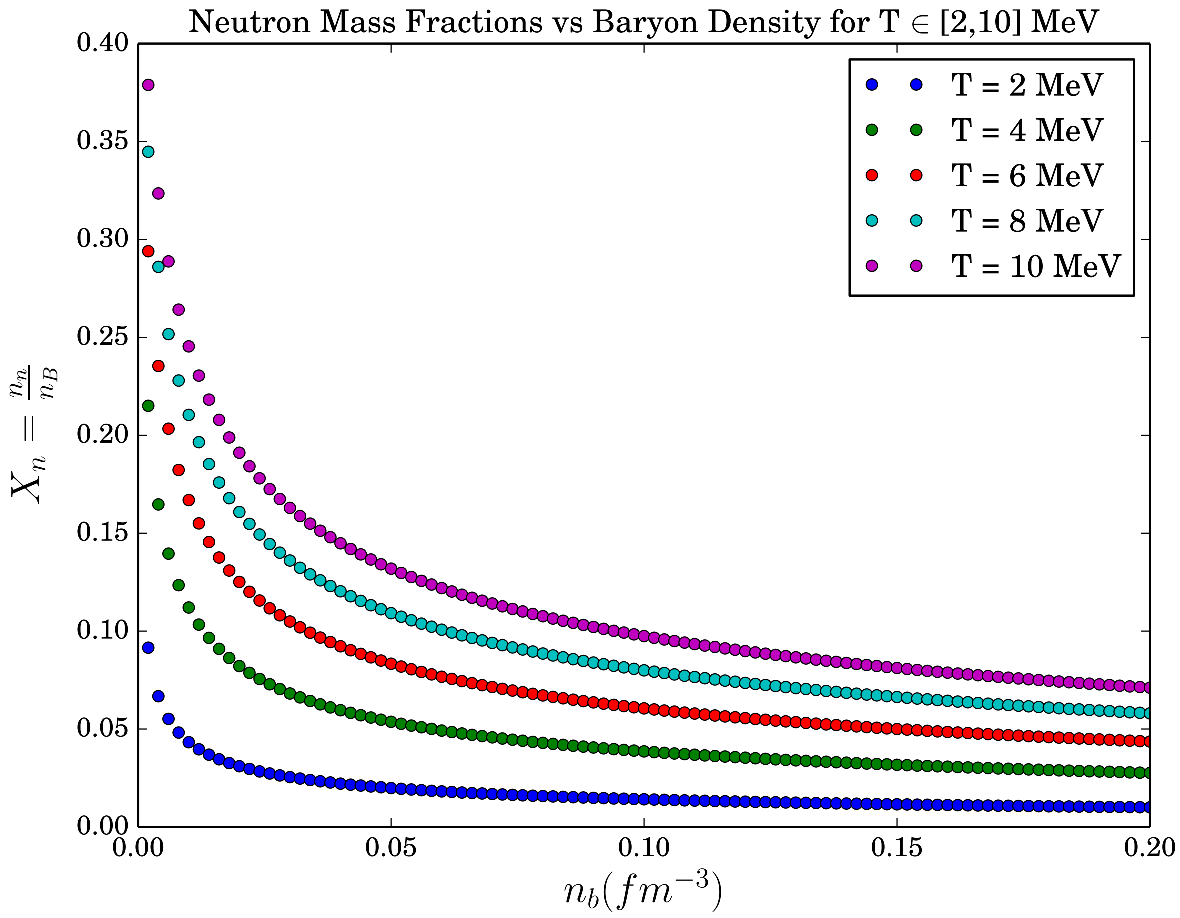

Figure 12. n_n Mass Fraction vs Baryon Density for point particles within $T \in [2, 10] MeV$.

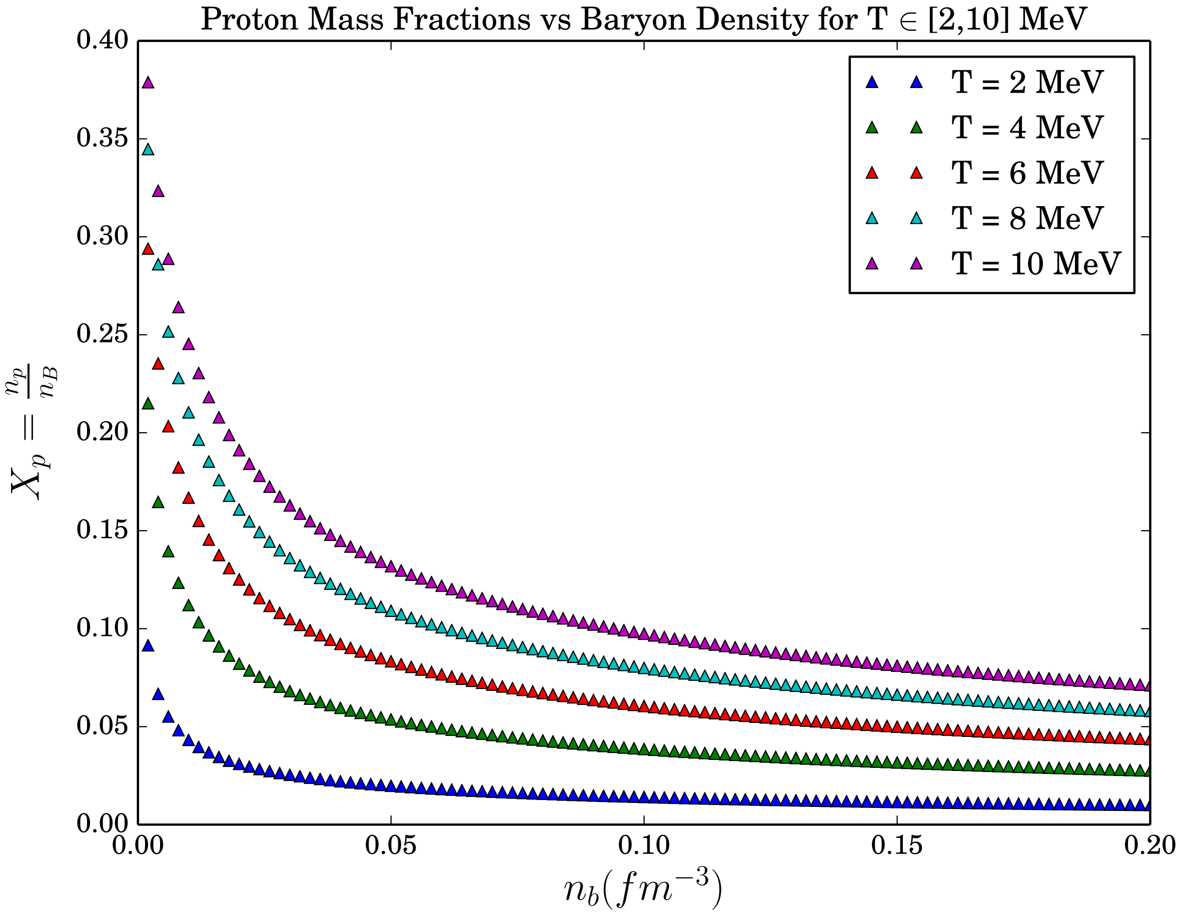

Figure 13. n_p Mass Fraction vs Baryon Density for point particles within $T \in [2, 10] MeV$.

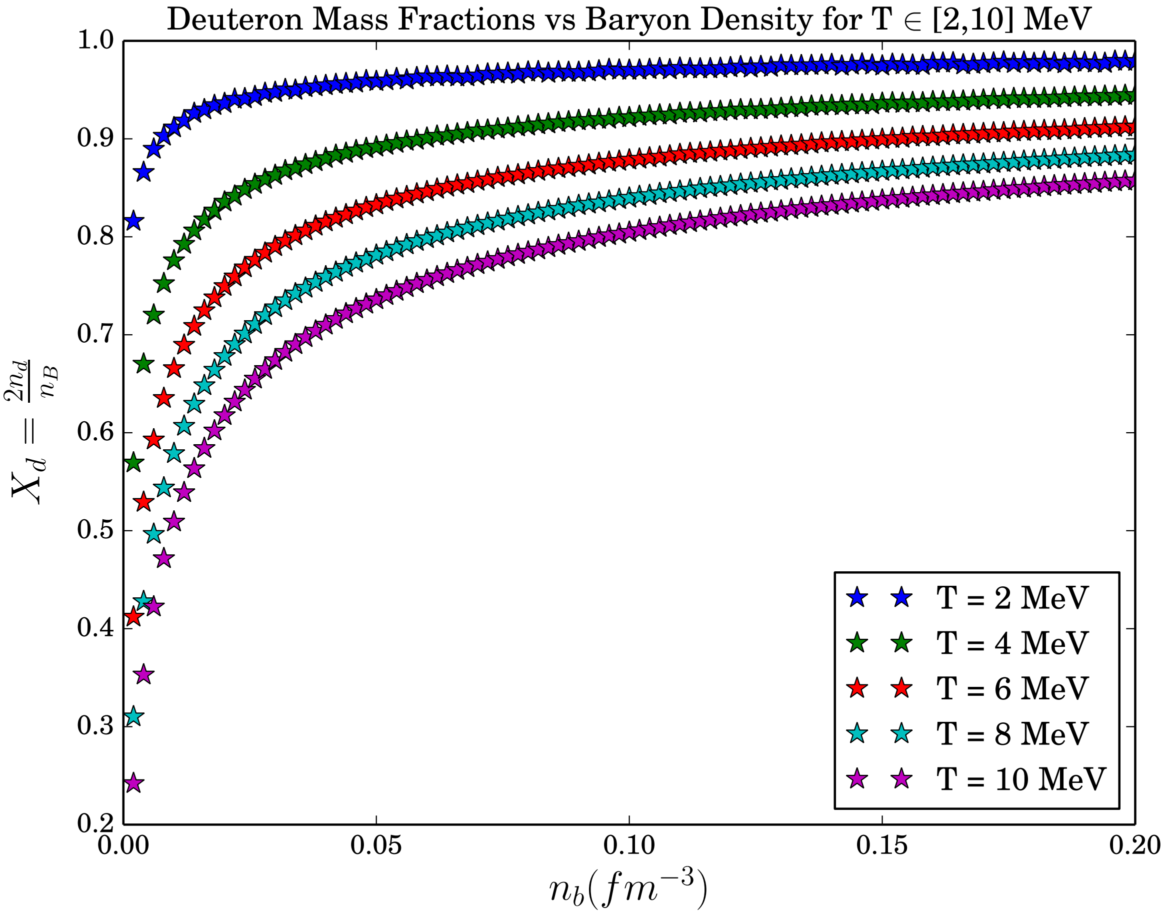

Figure 14. n_d Mass Fraction vs Baryon Density for point particles within $T \in [2, 10] MeV$.

Finite Non-zero Radii Particles ($R_i > 0$ (i = n, p, d))

In this case, we assume that deuteron has a finite radius $R_d = 1.2fm$

Table 2
Particle Pairs Volumes

Particle Pair	Volume (fm^3)
$v_{nn} = v_{pp}$	2.094
$v_{pn} = v_{np}$	2.094
$v_{dn} = v_{nd}$	7.238
$v_{pd} = v_{dp}$	7.238
v_{dd}	57.906

where

$$v_{dn} = v_{nd} = v_{dp} = v_{pd} = \frac{4\pi}{3} R_d^3 = 7.238 \ fm^3, \tag{3.24}$$

and

$$v_{dd} \approx \frac{4\pi}{3} (2R_d)^3 = 57.906 \ fm^3. \tag{3.25}$$

Using these terms we can introduce the rearrangement potentials into the number densities

$$U_i = -\sum_j v_{ij} \frac{\Omega_j^{(ex)}}{V\Phi_j}, \tag{3.26}$$

hence

$$U_i = -\sum_j v_{ij} \frac{\Omega_j^{(ex)}}{V\Phi_j} \Omega_i^{(ex)} = -TV \frac{g_i^{(eff)}\Phi_i}{\lambda_i^3} \exp\left(\frac{\mu_i^{(ex)} - m_i - U_i}{T}\right). \tag{3.27}$$

Combining these last two equations, we express the potentials more simply as

$$U_i = T \sum_j v_{ij} \frac{g_j}{\lambda_i^3} \exp\left(\frac{\mu_i^{(ex)} - m_i - U_i}{T}\right) = T \sum_j v_{ij} \frac{n_j}{V\Phi_j}. \tag{3.28}$$

And, using this, we can finally include volume-exclusion in our calculation of the particle densities

$$n_i = \frac{g_i^{(eff)}}{\lambda_i^3} \exp\left(\frac{\mu_i^{(ex)} - m_i - U_i}{T}\right) \tag{3.29}$$

$$= \frac{g_i\Phi_i}{\lambda_i^3} \exp\left(\frac{\mu_i^{(ex)} - m_i - U_i}{T}\right), \tag{3.30}$$

the results of which are shown in figures (15), (16), and (17).

Comparing these to Figures (12), (13), and (14) for the point particles, we have a vastly different scenario. Having considered volume exclusion, Figures (15), (16), and (17) suggest that we get a decrease in deuteron mass fraction as the baryon density increases. And, as temperature increases deuteron mass fraction decreases.

As in the previous case for point particles, the trend of neutrons and protons against the deuterons is reversed. But this time, the proton and neutron

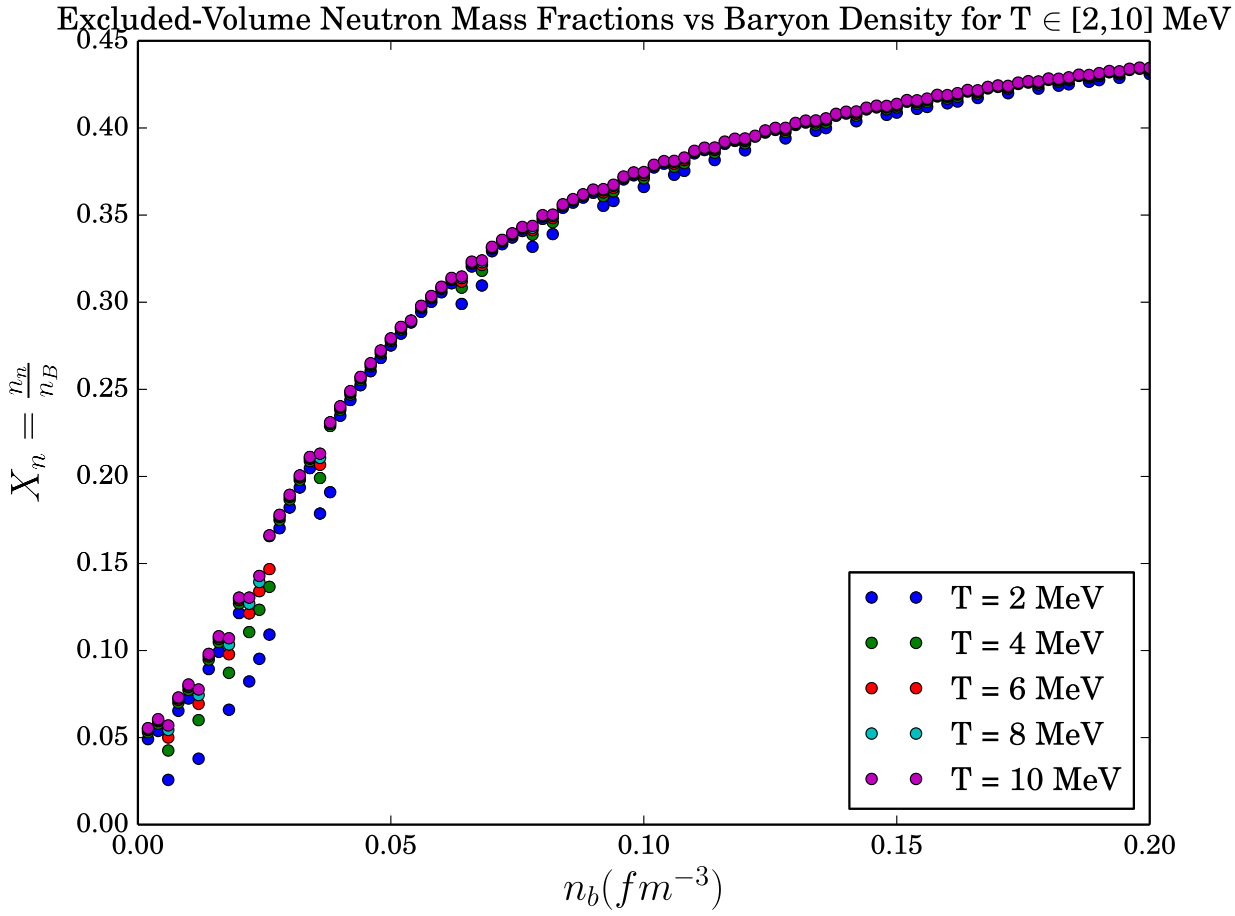

Figure 15. n_n Mass Fraction vs Baryon Density for volume-excluded particles within $T \in [2, 10] MeV$.

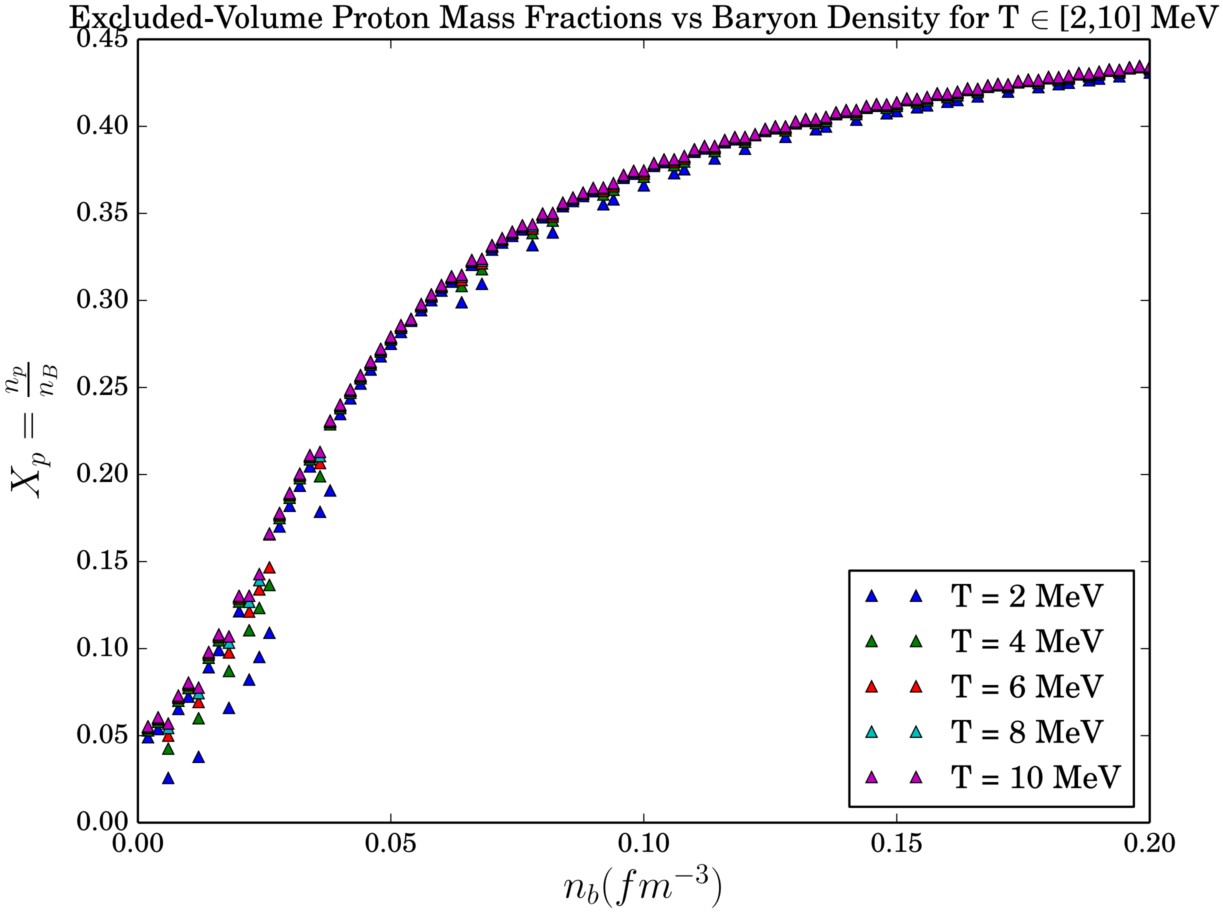

Figure 16. n_p Mass Fraction vs Baryon Density for volume-excluded particles within $T \in [2, 10] MeV$.

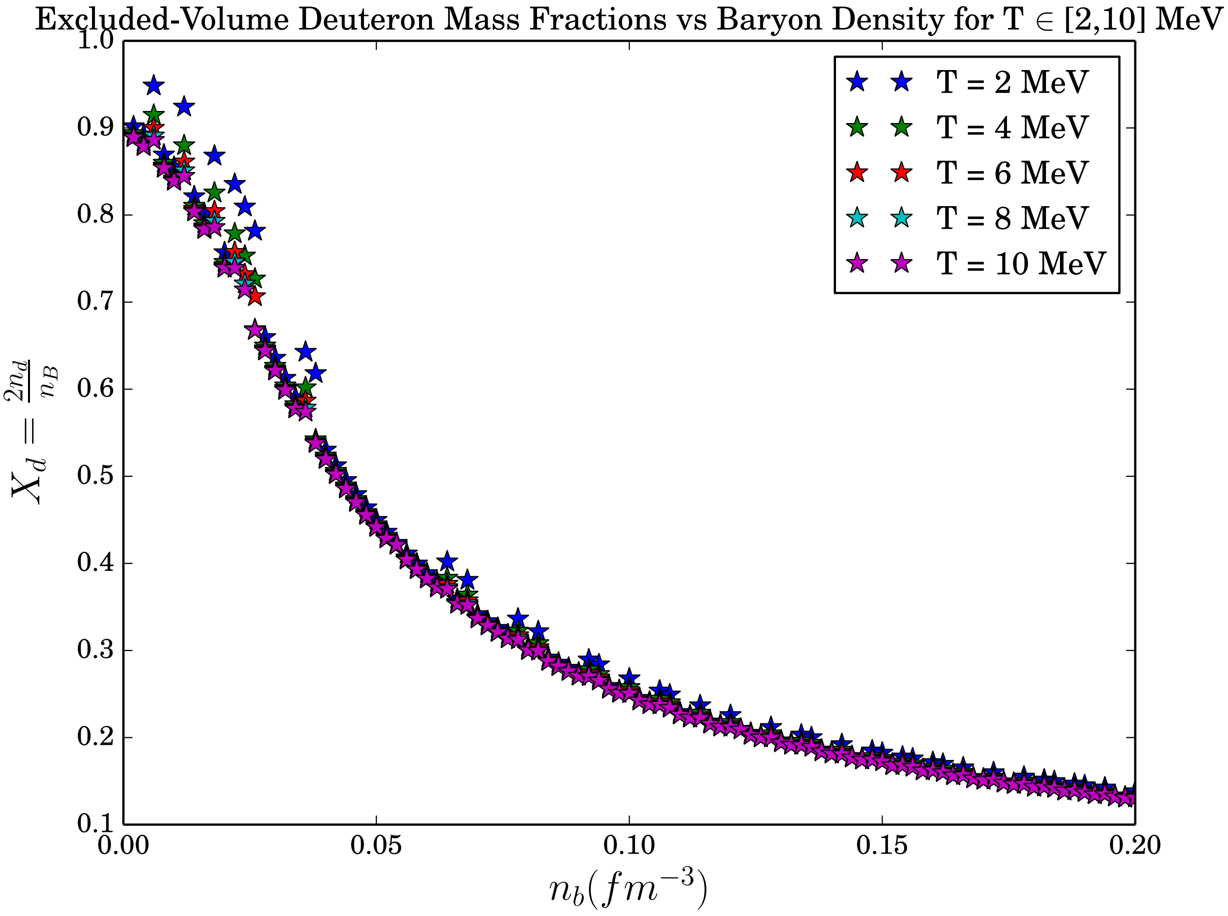

Figure 17. n_d Mass Fraction vs Baryon Density for volume-excluded particles within $T \in [2, 10] MeV$.

mass fractions increase with baryon density, and also for increasing temperature.

Future Work

Hence, while the results presented in this chapter are for the special case of a symmetric mixture of nucleons (i.e. $\delta = 0$) for three particle species, neutrons, protons and deuterons, this methodology should be applied and compared against actual data for different nuclei species to confirm its validity. Furthermore, more realistic consideration involving particle number conservation, non-conserved chemical potential, and energy loss or gain, and inclusion of relativistic physical situations should also be considered.

However, while such an approach is beyond the scope of this study, the arguments and approach made herein can be extended and applied in a more general sense beyond a finite mixture of gases of simple nucleons - as we have shown here.

Chapter 4

APPLICATIONS TO BIG BANG NUCLEOSYNTHESIS

We also note that this methodology - with the inclusion of relativity - can be applied to understanding Big Bang Nucleosynthesis. Additional but unrelated work to the one shown herein, was done with a collaboration with Prof. Spitaleri and his nuclear astrophysics group in Catania, Sicily as shown in Pizzone et al. (2014), the abstract of which is cited below.

"Nuclear reaction rates are among the most important input for understanding the primordial nucleosynthesis and therefore for a quantitative description of the early Universe. An up-to-date compilation of direct cross sections of ^{2}H(d,p) ^{3}H, ^{2}H(d,n) ^{3}He, ^{7}Li(p,α) ^{4}He and ^{3}He(d,p) ^{4}He reactions is given. These are among the most uncertain cross sections used and input for Big Bang nucleosynthesis calculations. Their measurements through the Trojan Horse Method (THM) are also reviewed and compared with direct data. The reaction rates and the corresponding recommended errors in this work were used as input for primordial nucleosynthesis calculations to evaluate their impact on the ^{2}H, ^{3,4}He and ^{7}Li primordial abundances, which are then compared with observations."

APPENDICES

APPENDIX A

CALCULATION OF b_{nn}

CALCULATION OF b_{nn}

From eq. (2.22)

$$p^{(vi,cl)} = -\frac{\Omega^{(vi,cl)}(T,V,\mu_n^{(vi,cl)})}{V} = \frac{T}{\lambda_n^3}\left[g_n z_n^{(vi,cl)} + b_{nn}^{(cl)}\left(z_n^{(vi,cl)}\right)^2\right], \tag{4.1}$$

and

$$p^{(vi,qu)} = -\frac{\Omega^{(vi,qu)}(T,V,\mu_n^{(vi,qu)})}{V} = \frac{T}{\lambda_n^3}\left[g_n z_n^{(vi,qu)} + b_{nn}^{(qu)}\left(z_n^{(vi,qu)}\right)^2\right], \tag{4.2}$$

we have

$$n_n = \frac{\partial p^{(vi,cl)}}{\partial \mu_n} = \frac{1}{\lambda_n^3}\left[g_n z_n^{(vi,cl)} + 2b_{nn}^{(cl)}\left(z_n^{(vi,cl)}\right)^2\right], \tag{4.3}$$

and

$$n_n = \frac{\partial p^{(vi,qu)}}{\partial \mu_n} = \frac{1}{\lambda_n^3}\left[g_n z_n^{(vi,qu)} + 2b_{nn}^{(qu)}\left(z_n^{(vi,qu)}\right)^2\right]. \tag{4.4}$$

Simplifying this, we arrive at the relations

$$n_n = \frac{1}{\lambda_n^3}\left[g_n z_n^{(vi)} + 2b_{nn}\left(z_n^{(vi)}\right)^2\right], \tag{4.5}$$

$$n_n\lambda_n^3 = g_n z_n^{(vi)} + 2b_{nn}\left(z_n^{(vi)}\right)^2, \tag{4.6}$$

leading to

$$\left(z_n^{(vi)}\right)^2 + z_n^{(vi)}\frac{g_n}{2b_{nn}} - \frac{n_n\lambda_n^3}{2b_{nn}} = 0, \tag{4.7}$$

which has the solution:

$$z_n^{(vi)} = \frac{1}{4b_{nn}}\left(\pm\sqrt{g_n^2 + 8b_{nn}n_n\lambda_n^3} - g_n\right). \tag{4.8}$$

Hence, inserting into eqs. (4.1) and (4.2) respectively

$$\begin{aligned}
p^{(vi)} &= \frac{T}{\lambda_n^3}\left[g_n z_n^{(vi)} + b_{nn}\left(z_n^{(vi)}\right)^2\right], \\
&= \frac{T}{\lambda_n^3}\left[g_n z_n^{(vi)} + b_{nn}\left(\frac{n_n\lambda_n^3}{2b_{nn}} - z_n^{(vi)}\frac{g_n}{2b_{nn}}\right)\right], \\
&= \frac{T}{\lambda_n^3}\left[g_n z_n^{(vi)} + \frac{1}{2}\left(n_n\lambda_n^3 - g_n z_n^{(vi)}\right)\right], \\
&= \frac{T}{2\lambda_n^3}\left[g_n z_n^{(vi)} + n_n\lambda_n^3\right], \\
&= \frac{T}{2\lambda_n^3}\left[n_n\lambda_n^3 + g_n\left(\pm\sqrt{g_n^2 + 8b_{nn}n_n\lambda_n^3} - g_n\right)\right], \\
&= \frac{T}{2\lambda_n^3}\left[n_n\lambda_n^3 - g_n^2 \pm \sqrt{g_n^4 + 8g_n^2 b_{nn}n_n\lambda_n^3}\right].
\end{aligned} \tag{4.9}$$

To produce real values for $p^{(vi)}$ we must have the condition (constraint to b_{nn})

$$g_n^4 \geq -8 g_n^2 b_{nn} n_n \lambda_n^3, \tag{4.10}$$

or

$$\frac{g_n^2}{8\lambda_n^3 n_n} \geq -b_{nn}. \tag{4.11}$$

For the classical case for neutrons, this is:

$$b_{nn}^{(cl)}(T) = -\frac{g_n^2}{\lambda_n^3}\frac{4\pi}{3}R_{nn}^3, \tag{4.12}$$

or

$$\frac{g_n^2}{8\lambda_n^3 n_n} \geq +\frac{g_n^2}{\lambda_n^3}\frac{4\pi}{3}R_{nn}^3. \tag{4.13}$$

Thus, the limiting density is

$$\frac{g_n^2}{8\lambda_n^3 n_n} \geq \frac{g_n^2}{\lambda_n^3}\frac{4\pi}{3}R_{nn}^3, \tag{4.14}$$

or

$$\frac{1}{8n_n} \geq \frac{4\pi}{3} R_{nn}^3. \tag{4.15}$$

In terms of the neutron number density (and recalling that $R_{nn} \approx 1fm$)

$$\frac{3}{32\pi}\frac{1}{R_{nn}^3} \geq n_n \approx 0.029842\, fm^{-3}, \tag{4.16}$$

the excluded volume is

$$v_{nn} = \frac{1}{2}\frac{4\pi}{3} R_{nn}^3, \tag{4.17}$$

leading to

$$\frac{3}{32\pi}\frac{1}{R_{nn}^3} \to \frac{1}{16v_{nn}} \geq n_n \approx 0.029842\, fm^{-3}. \tag{4.18}$$

Noticeably, this is temperature independent and is only constrained to the the volume of the sphere in question - i.e. volume dependent - as it should be.

For the quantum mechanical case

$$b_{nn}^{(vi,qm)}(T) = \sum_{l=0}^{l=\infty} b_{nn}^{(l)}(T), \tag{4.19}$$

thus, using

$$b_{nn}^{(l)}(T) = \frac{(2l+1)g_n^2}{\pi} \frac{\lambda_n^3}{\lambda_{nn}^3} \int_0^\infty \exp\left(-\frac{k^2}{2\mu_{nn}T}\right) \frac{d\delta_l^{(ij)}}{dk}, \tag{4.20}$$

we obtain

$$b_{nn}^{(vi,qm)}(T) = \sum_{l=0}^{l=\infty} b_{nn}^{(l)}(T), \tag{4.21}$$

where

$$\frac{g_n^2}{8\lambda_n^3 n_n} \geq -\sum_{l=0}^{l=\infty} b_{nn}^{(l)}(T). \tag{4.22}$$

Defining the integration result as *f(T)*, we have

$$b_{nn}^{(vi,qm)}(T) = \sum_{l=0}^{l=\infty} \frac{(2l+1)g_n^2}{\pi} \frac{\lambda_n^3}{\lambda_{nn}^3} f(T) = \frac{(2l+1)g_n^2}{\pi} \frac{\lambda_n^3}{\lambda_{nn}^3} \sum_{l=0}^{l=\infty} f(T), \tag{4.23}$$

since

$$\frac{g_n^2}{8\lambda_n^3 b_{nn}^{(vi,qm)}(T)} \geq n_n, \tag{4.24}$$

we get

$$\frac{g_n^2}{8\lambda_n^3 \frac{g_n^2}{\pi} \frac{\lambda_n^3}{\lambda_{nn}^3}} \geq n_n \sum (2l+1) f(T), \tag{4.25}$$

or

$$\frac{\pi g_n^2 \lambda_{nn}^3}{8\lambda_n^3 g_n^2 \lambda_n^3} \geq n_n \sum (2l+1) f(T), \tag{4.26}$$

that is

$$\frac{\pi \lambda_{nn}^3}{8\lambda_n^6 \sum (2l+1) f(T)} \geq n_n. \tag{4.27}$$

From an examination of the terms, we observe that $\sum(2l+1)f(T)$ requires that the overall integrand result be unitless, so that it can be thought of as a single function dependent on T. Hence at a given temperature and nucleon density, we can write

$$\frac{\pi \lambda_{nn}^3}{8\lambda_n^6 n_n} \geq \sum (2l+1) f(T). \tag{4.28}$$

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