Virial Coefficients of 3-Flavor Fermionic Systems with Three-Body Contact Interactions in the Lattice Semi-Classical Approximation at Leading Order

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April 2019

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1 Introduction

Many of the interactions in classical and quantum systems are in the form of two-body forces, or sums of these forces. Electric and magnetic forces for example can be found by summing all the two-body forces between one body and all others. In some systems however, there are interactions that exist only when three particles are together, or forces that are non-additive. These forces appear more exotic, but come naturally in several scenarios (7)(4)(5)(1). Also, three-body forces are possible in ultracold systems in an Efimov state, where trimers (triangular three-body bound states) form when two-body states are unbound (6) (3).

Some unique systems like Efimov states may have only three-body forces, while other could have a combination of two and three-body forces. This project focused on characterizing the three-body forces exclusively as two-body systems are already being studied by the group.

Besides understanding the dynamics of these systems, which could be extraordinarily complex, one can ask questions about the thermal properties. How does a three-body system respond to changes in temperature or pressure? To answer this, one must find a way to extract the thermal properties of the system. One approach is the ideal gas law, however, complex quantum systems are unlikely to fit under the constraints of an ideal gas, so some corrections have to be made. The grand-canonical ensemble is one which can exchange heat and particles with the environment, which describes the system in which we will work. The advantage of dealing with this ensemble is that the grand-potential contains information about the thermal properties of the system. We must now look for away to connect the statistical description to the properties of the dilute gas

The virial expansion is a correction to the ideal gas law from which thermal properties can be found. The virial coefficients are coefficients of the Taylor expansion of the grand-canonical partition function in terms of the chemical potential, more specifically, fugacity. The expanision is non-perturbative and valid in the dilute limit (8) The goal is to calculate individual coefficients to powers of the fugacity. Each increase in the order of the fugacity contains information relative N-body partition function. The difficulty lies in calculating these coefficients, which are often associated with solving the N-body problem, particularly difficult because the number of terms scales as $N!^2$. This can be addressed by rewriting Slater determinants as sums over permutations and carefully proceeding on paper, or using symbolic algebra programs. Both Mathematica and FORM are capable of doing the calculation, however, after some experiment, FORM code is much more efficient and more suitable for the calculation rewritten as contractions over Levi-Civita tensors and delta functions. A text editing process extracts the relevant terms. Processing the data is challenging because there are a number of terms that look like Kroenecker delta functions of three or more terms, for which we could not find built in methods for simplifying these terms, so network analysis techniques can be used to construct graphs and simply the expressions to a more manageable form.

2 Theory

2.1 Virial Expansion

Ultimately we are interested in characterizing thermal properties of quantum few body systems through statistical mechanics. The objects of interest for this systems are the grand-canonical partition function Z and the grand-potential Ω. All the information for the system is contained withing the partition function and the potential, and from them, various thermal properties can be calculated. We will work in units where $\hbar = k_B = 1$. Beginning with the grand-canonical partition function

$$Z = \sum_{n=0}^{\infty} e^{-\beta(E_n - \mu N_n)}, \tag{1}$$

where β is inverse temperature ($\frac{1}{k_B T}$and μ is the chemical potential. We do not yet have this information, however, so we will need to calculate Z in terms of operators as

$$Z = \mathrm{Tr}[e^{-\beta(\hat{H} - \mu\hat{N})}]. \tag{2}$$

Since our Hamiltonian has no effect on the number of particles ($[\hat{H}, \hat{N}] = 0$), using 1 we can separate the grand-canonical part and write Z in powers of the fugacity, $z = e^{\beta\mu}$

$$Z = \sum_{n=0}^{\infty} Q_n z^n, \tag{3}$$

where Q_n are the n-body canonical partition functions. More explicitly, the one-body canonical partition function is

$$Q_{100} = e^{-\beta E}. \tag{4}$$

In the above, the exact form of E varies according to the system. For a Fermi gas, $E = p^2/2m$. A series expansion in fugacity assumes a dilute gas, however the fugacity can be made small by a number of means. Now that we have a direction to follow for the calculations, we must connect this to thermal properties. The grand potential is

$$\Omega = U - TS - \mu N \tag{5}$$

where U is the internal energy, T is the temperature, S is the entropy, and μ is still the chemical potential. Thus, for our system,

$$\Omega = PV. \tag{6}$$

where P is pressure, and V is the spatial volume in any dimension (important as one can go quite far before specifying the dimensions of the system). Using the important relation,

$$-\beta\Omega = \ln Z. \tag{7}$$

We then expand in powers of the fugacity z

$$-\beta\Omega = \ln Z = Q_1 \sum_{n=1}^{\infty} b_n z^n \tag{8}$$

where b_n are virial coefficients. Using (3) and (8), we can Taylor expand $\ln Z$ and group in terms of Q_n:

$$\begin{aligned}
\ln Z = Q_1 \Bigg[& z + \left(\frac{Q_2}{Q_1} - \frac{Q_1}{2}\right) z^2 + \left(\frac{Q_1^2}{3} - Q_2 + \frac{Q_3}{Q_1}\right) z^3 + \\
& \left(-\frac{Q_1^3}{4} + Q_2 Q_1 - Q_3 - \frac{Q_2^2}{2Q_1} + \frac{Q_4}{Q_1}\right) z^4 + \\
& \left(\frac{Q_1^4}{5} - Q_2 Q_1^2 + Q_3 Q_1 + Q_2^2 - Q_4 - \frac{Q_2 Q_3}{Q_1} + \frac{Q_5}{Q_1}\right) z^5 + \\
& \Bigg(- \frac{Q_1^5}{6} + Q_2 Q_1^3 - Q_3 Q_1^2 - \frac{3}{2} Q_2^2 Q_1 + Q_4 Q_1 + \\
& 2 Q_2 Q_3 - Q_5 + \frac{Q_2^3}{3Q_1} - \frac{Q_3^2}{2Q_1} - \frac{Q_2 Q_4}{Q_1} + \frac{Q_6}{Q_1}\Bigg) z^6 + \\
& \Bigg(\frac{Q_1^6}{7} - Q_2 Q_1^4 + Q_3 Q_1^3 + 2 Q_2^2 Q_1^2 - Q_4 Q_1^2 - 3 Q_2 Q_3 Q_1 + Q_5 Q_1 - \\
& Q_2^3 + Q_3^2 + 2 Q_2 Q_4 - Q_6 + \frac{Q_2^2 Q_3}{Q_1} - \frac{Q_3 Q_4}{Q_1} - \frac{Q_2 Q_5}{Q_1} + \frac{Q_7}{Q_1}\Bigg) z^7 + \\
& \Bigg(- \frac{Q_1^7}{8} + Q_2 Q_1^5 - Q_3 Q_1^4 - \frac{5}{2} Q_2^2 Q_1^3 + Q_4 Q_1^3 + 4 Q_2 Q_3 Q_1^2 - Q_5 Q_1^2 + 2 Q_2^3 Q_1 - \\
& \frac{3}{2} Q_3^2 Q_1 - 3 Q_2 Q_4 Q_1 + Q_6 Q_1 - 3 Q_2^2 Q_3 + 2 Q_3 Q_4 + 2 Q_2 Q_5 - Q_7 - \\
& \frac{Q_2^4}{4Q_1} + \frac{Q_2 Q_3^2}{Q_1} - \frac{Q_4^2}{2Q_1} + \frac{Q_2^2 Q_4}{Q_1} - \frac{Q_3 Q_5}{Q_1} - \frac{Q_2 Q_6}{Q_1} + \frac{Q_8}{Q_1}\Bigg) z^8 + ... \Bigg]
\end{aligned}$$

This rather intimidating expression contains the information about how additional particles and interactions within a system contribute to the partition, and by definition, the energy spectrum and thermodynamics.

Collecting the factors (in large parenthesis) in front of each order of fugacity, we have the virial coefficients, b_n. Here ends the most general form of the virial expansion as we have not yet specified the interactions. Adding in the interactions, and removing non interacting physics, we will have expressions representing Δb_n and ΔQ_N.

2.2 Three-Body Contact interactions

Proceeding with three-body interactions, we can define the partition functions we need to calculate accounting for symmetry across 3 flavors of otherwise identical fermions as

$$Q_3 = Q_{111}, \tag{9}$$
$$Q_4 = 3Q_{211}, \tag{10}$$
$$Q_5 = 3Q_{311} + 3Q_{221}, \tag{11}$$
$$Q_6 = 3Q_{411} + 6Q_{321} + Q_{222}, \tag{12}$$
$$Q_7 = 3Q_{511} + 6Q_{421} + 3Q_{322}, \tag{13}$$
$$Q_8 = 3Q_{611} + 6Q_{521} + 6Q_{431} + 3Q_{422} + 3Q_{332}, \tag{14}$$

where the expression Q_{LMN} represents the partition function of a system with L fermions of flavor A, M of flavor B, and N of flavor C. While this language is suggestive of QCD, this is not necessarily the system in question: the word 'flavor' is used as a synonym of 'fermion species'. The calculation assumes a non-relativistic system, where the particle number is conserved. In a relativistic system, we would replace number with charge, which could be positive or negative.

As we will see later, the three-body partition functions defined above are the ones of interest in relation to the virial expansion. We will be calculating the change in the partition functions, , ΔQ, when interactions are turned on, therefore ΔQ's without an interaction will be zero. Explicitly, any ΔQ_{LMN} must have L,M and N non-zero to remain, for example, $\Delta Q_{330} = 0$. Also since we are only using three-body interactions with all three species present, $\Delta Q_1 = \Delta Q_2 = 0$.

Further, we use the Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}. \tag{15}$$

The potential operator for three-body contact interactions is

$$\hat{V} = -g \sum_x \hat{n_1}(x)\hat{n_2}(x)\hat{n_3}(x), \tag{16}$$

where $\hat{n_s}(x)$ is the number operator for fermion species s at position x. Thus, the potential is zero unless all three species are present at one lattice site.

For Fermi gasses the action of the kinetic energy operator will yield terms of the form

$$e^{-\beta\epsilon(p)} = e^{-\beta p^2/2m}. \tag{17}$$

2.3 Lattice Semi-Classical Approximation

For clarity, at this point spacetime has been discretized on a lattice. At the cost of a *chance* of an exact solution, this has the tremendous advantage that discrete systems can be immediately treated on a computer. In theory we could increase the number of lattice points and decrease the spacing until we reach the continuum limit. This calculation was performed without numerical methods however, so we will not pursue this further other than suggesting that an excellent way of confirming these results would be to match them to numerical results. In the grand-canonical ensemble, we seek to evaluate expressions with the operator

$$e^{-\beta(\hat{H}+\mu\hat{N})}. \tag{18}$$

The expansion in fugacity leaves us with the Hamiltonian,

$$\hat{H} = \hat{T} + \hat{V}, \tag{19}$$

where $\hat{T}$ and $\hat{V}$ are the kinetic and potential energy operators, respectively. The richness of quantum mechanics lies in the non-commuting nature of these two operators, which is where the LSCA comes in. We use the Trotter-Suzuki factorization (9). This is a specific case of a generalized Lie product.

$$e^{-\beta\hat{T}-\beta\hat{V}} = e^{-\beta\hat{T}}e^{-\beta\hat{V}}e^{-\frac{\beta^2}{2}\hat{T}}e^{-\frac{\beta^2}{2}\hat{V}}... \tag{20}$$

In the lowest order approximation, we use only terms linear in β. In the strong or weak coupling limits, we can ignore either $\hat{T}$ or $\hat{V}$ respectively, so the assumption that $[\hat{T}, \hat{V}] = 0$ becomes exact. Although the rest of the work is done at leading order, it is possible to continue to higher orders in the TS factorization. This is of interest for further exploration. Although the term TS is normally reserved for numerical work, the leading order can be considered as a coarse TS factorization with timestep $\tau = \frac{\beta}{n}$ with $n = 1$.

3 Three-Body Contact Potential

We will walk through the calculation of a relatively simple and then slightly more complex term to demonstrate the calculation and the need for digital assistance.

3.1 Q_{111} for Δb_3

We wish to evaluate Δb_3 which is

$$\Delta b_3 = \frac{\Delta Q_{111}}{Q_{100}}$$

Using TS-factorization and using shorthand p for all momenta in the sum and similarly for the state vector

$$Q_{111} = \sum_{p_1,p_2,p_3,} \langle \mathbf{p_1 p_2 p_3} | e^{-\beta(\hat{T}+\hat{V})} | \mathbf{p_1 p_2 p_3} \rangle = \sum_{p} \langle \overline{\mathbf{p}} | e^{-\beta \hat{T}} e^{-\beta \hat{V}} | \overline{\mathbf{p}} \rangle$$

where we are summing over all momentum states. Acting the kinetic energy operator is simple in this basis and we do so first

$$Q_{111} = \sum_{p} e^{-\beta({p_1}^2+{p_2}^2+{p_3}^2 w)/2m} \langle \overline{\mathbf{p}} | e^{-\beta \hat{V}} | \overline{\mathbf{p}} \rangle$$

Again using shorthand $\epsilon_n = {p_n}^2/2m$ where ϵ is the sum over all ϵ_n, we insert a complete set of states

$$Q_{111} = \sum_{\substack{p \\ x_1,x_2,x_3}} e^{-\beta\epsilon} \langle \overline{\mathbf{p}} | e^{-\beta \hat{V}} | \overline{\mathbf{x}} \rangle \langle \overline{\mathbf{x}} | \overline{\mathbf{p}} \rangle$$

Where each x term is summing over all space. Noting that $\hat{V} = -g \sum_x \hat{n_1}(x)\hat{n_2}(x)\hat{n_3}(x)$ and for fermions ${\hat{n_s}}^2 = \hat{n_s}$

$$e^{-\beta \hat{V}} | \overline{\mathbf{x}} \rangle = (1 - \beta \hat{V} + \beta^2 \hat{V}^2 - \beta^3 \hat{V}^3 + ...) | \overline{\mathbf{x}} \rangle$$

In the Q_{111} case, the result of the sum enforcing the contact interaction in $\hat{V}$ gives

$$\begin{aligned} &\delta(x_1 - z)\delta(x_2 - z)\delta(x_3 - z) | \overline{\mathbf{x}} \rangle \\ &= \delta(x_1 - x_2)\delta(x_1 - x_3) | \overline{\mathbf{x}} \rangle = f_1 | \overline{\mathbf{x}} \rangle \end{aligned}$$

Which allows us to rewrite the Taylor expansion and simplify, noting that $f_1^2 = f_1$ as only one interaction can happen at once with 3 particles. One can separate the non interacting term, which we drop to calculate ΔQ_{111}

$$Q_{111} = [1 + (\beta g f_1 + \beta^2 g^2 f_1 + \beta^3 g^3 f_1 + ...)] | \overline{\mathbf{x}} \rangle = [1 + (e^{\beta g} - 1) f_1] | \overline{\mathbf{x}} \rangle$$

Using the shorthand $C = (e^{\beta g} - 1)$ and summing over delta function, the calculation now becomes

$$\Delta Q_{111} = C \sum_{\substack{p \\ x_1, x_2, x_3}} e^{-\beta\epsilon} f_1 |\langle \overline{\mathbf{x}} | \overline{\mathbf{p}} \rangle|^2 = C \sum_{\substack{p \\ x_1}} e^{-\beta\epsilon} |\langle \overline{\mathbf{x}} | \overline{\mathbf{p}} \rangle|^2$$

Since we have no identical particles, the inner product is straightforward

$$\Delta Q_{111} = C \sum_{\substack{p_1, p_2, p_3 \\ x_1}} e^{-\beta\epsilon} |\langle \mathbf{x_1 x_2 x_3} | \mathbf{p_1 p_2 p_3} \rangle|^2$$

$$\Delta Q_{111} = C \sum_{\substack{p_1, p_2, p_3 \\ x_1}} e^{-\beta\epsilon} \frac{1}{1!1!1!} \left| \frac{e^{ip_1 x_1}}{\sqrt{V}} \frac{e^{ip_2 x_2}}{\sqrt{V}} \frac{e^{ip_3 x_3}}{\sqrt{V}} \right|^2$$

$$\Delta Q_{111} = C \sum_{\substack{p_1, p_2, p_3 \\ x_1}} e^{-\beta\epsilon} \frac{1}{V^3}$$

Now summing over x_1 contributes a factor of the volume

$$C \sum_{\substack{p_1, p_2, p_3 \\ x_1}} e^{-\beta\epsilon} \frac{1}{V^3} = \frac{C}{V^3} \sum_{p_1, p_2, p_3} e^{-\beta\epsilon} V$$

One can recognize the quantity as the 1-body partition function cubed, which we continue with in our expression for Δb_3

$$\Delta Q_{111} = \frac{C}{V^2} \sum_{p_1, p_2, p_3} e^{-\beta {p_1}^2/2m} e^{-\beta {p_2}^2/2m} e^{-\beta {p_3}^2/2m} = \frac{C}{V^2} Q_{100}^3$$

$$\Delta b_3 = \frac{\Delta Q_{111}}{Q_1} = C \frac{Q_{100}^3}{3 Q_{100} V^2} = (e^{\beta g} - 1) \frac{Q_{100}^2}{3V^2}$$

3.2 Q_{222} for Δb_6

Moving on to a more complex example, one can notice looking at the calculations up to Δb_6, that in we still have not yet had multiple interactions. Additionally, this is the first calculation that does not resemble the two body case. Specifically, for Δb_6 we have the term Q_{222} which has exactly two simultaneous interactions. We begin as usual writing out the explicit form of the calculation

$$\begin{aligned} Q_{222} &= \sum_{p_1, p_2, p_3, p_4, p_5, p_6} \langle \mathbf{p_1 p_2 p_3 p_4 p_5 p_6} | e^{-\beta(\hat{T} + \hat{V})} | \mathbf{p_1 p_2 p_3 p_4 p_5 p_6} \rangle \\ &= \sum_{p} \langle \overline{\mathbf{p}} | e^{-\beta \hat{T}} e^{-\beta \hat{V}} | \overline{\mathbf{p}} \rangle \end{aligned}$$

Acting $\hat{T}$ we get

$$= \sum_p e^{-\beta({p_1}^2+{p_2}^2{p_3}^2+{p_4}^2+{p_5}^2+{p_6}^2)/2m} \langle \overline{\mathbf{p}}|e^{-\beta\hat{V}}|\overline{\mathbf{p}}\rangle = \sum_p e^{-\beta\epsilon} \langle \overline{\mathbf{p}}|e^{-\beta\hat{V}}|\overline{\mathbf{p}}\rangle$$

Now, we insert a complete set of states as before.

$$Q_{222} = \sum_{\substack{p \\ x}} e^{-\beta\epsilon} \langle \overline{\mathbf{p}}|e^{-\beta\hat{V}} |\overline{\mathbf{x}}\rangle \langle \overline{\mathbf{x}}| \overline{\mathbf{p}}\rangle$$

Which leads to a new factor in our expression for acting $\hat{V}$

$$e^{-\beta\hat{V}} |\overline{\mathbf{x}}\rangle = [1 - \beta\hat{V} + \beta^2\hat{V}^2 - \beta^3\hat{V}^3 + ...] |\overline{\mathbf{x}}\rangle$$

We now must consider higher orders of $\hat{V}$, as squaring the operator previously yielded only 1 set of viable position relations obeying the Pauli Exclusion Principle. Now, however, there will be a first order term enforcing one interaction, while the second order term will enforce two simultaneous interactions. With the shorthand $C = e^{\beta g_{dD}} - 1$ we can write this as

$$e^{-\beta\hat{V}} |\overline{\mathbf{x}}\rangle = [1 + \beta C f_1 + \beta^2 C^2 f_2] |\overline{\mathbf{x}}\rangle \tag{21}$$

where

$$\begin{aligned} f_1(\bar{\mathbf{x}}) = {} & \delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_1-\mathbf{x}_5)+\delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_1-\mathbf{x}_6) \\ & +\delta(\mathbf{x}_1-\mathbf{x}_4)\delta(\mathbf{x}_1-\mathbf{x}_5)+\delta(\mathbf{x}_1-\mathbf{x}_4)\delta(\mathbf{x}_1-\mathbf{x}_6) \\ & +\delta(\mathbf{x}_2-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_5)+\delta(\mathbf{x}_2-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_6) \\ & +\delta(\mathbf{x}_2-\mathbf{x}_4)\delta(\mathbf{x}_2-\mathbf{x}_5)+\delta(\mathbf{x}_2-\mathbf{x}_4)\delta(\mathbf{x}_2-\mathbf{x}_6) \end{aligned} \tag{22}$$

and

$$\begin{aligned} f_2(\bar{\mathbf{x}}) = f_1(\bar{\mathbf{x}}) + 2[& \delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_1-\mathbf{x}_5)\delta(\mathbf{x}_2-\mathbf{x}_4)\delta(\mathbf{x}_2-\mathbf{x}_6) \\ & +\delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_1-\mathbf{x}_6)\delta(\mathbf{x}_2-\mathbf{x}_4)\delta(\mathbf{x}_2-\mathbf{x}_5) \\ & +\delta(\mathbf{x}_1-\mathbf{x}_4)\delta(\mathbf{x}_1-\mathbf{x}_5)\delta(\mathbf{x}_2-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_6) \\ & +\delta(\mathbf{x}_1-\mathbf{x}_4)\delta(\mathbf{x}_1-\mathbf{x}_6)\delta(\mathbf{x}_2-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_5)] \end{aligned} \tag{23}$$

To evaluate $|\langle\bar{\mathbf{x}}|\bar{\mathbf{p}}\rangle|^2$ we must compute three 2×2 Slater determinants and multiply by the complex conjugate, resulting in 64 terms. Moving the volume factors out of the Slater determinants, we can write the inner product as

$$\begin{aligned} |\langle\bar{\mathbf{x}}|\bar{\mathbf{p}}\rangle|^2 &= \frac{1}{2!}\frac{1}{2!}\frac{1}{2!}\frac{1}{V^6}\left\|\begin{vmatrix} e^{ip_1x_1} & e^{ip_2x_1} \\ e^{ip_1x_2} & e^{ip_2x_2} \end{vmatrix}\begin{vmatrix} e^{ip_3x_3} & e^{ip_4x_3} \\ e^{ip_3x_4} & e^{ip_4x_4} \end{vmatrix}\begin{vmatrix} e^{ip_5x_5} & e^{ip_6x_5} \\ e^{ip_5x_6} & e^{ip_6x_6} \end{vmatrix}\right\|^2 \\ &= \frac{1}{8V^6}\left\|\begin{vmatrix} e^{ip_1x_1} & e^{ip_2x_1} \\ e^{ip_1x_2} & e^{ip_2x_2} \end{vmatrix}\begin{vmatrix} e^{ip_3x_3} & e^{ip_4x_3} \\ e^{ip_3x_4} & e^{ip_4x_4} \end{vmatrix}\begin{vmatrix} e^{ip_5x_5} & e^{ip_6x_5} \\ e^{ip_5x_6} & e^{ip_6x_6} \end{vmatrix}\right\|^2 \end{aligned}$$

Now, to get the linear order (1 interaction) result, we compute the determinant as is, but for higher orders of $\hat{V}$ we must consider the additional interactions

before computing the determinants, as given by f_1 and f_2. Fortunately, the result is symmetric across all terms of each function so we can simply proceed with one. While this number of particles is still manageable, there are terms produced such as

$$e^{((p_2-p_1)x_1+(p_1-p_2)x_2+(p_3-p_4)x_3+(p_4-p_3)x_4+(p_5-p_6)x_5+(p_6-p_5)x_6)} \tag{24}$$

which are rather unwieldy to work with by hand, making the symbolic algebra computation a much more attractive option. Further, considering the multiple interactions creates more exotic terms that are not easily described in terms of just the canonical partition functions. To this end we will dedicate a section entirely to dealing with higher orders of C, and for now focus on just 1 interaction at a time. Unlike the previous case, there are now a number of terms with different volume scaling, which we remove here for demonstration, the initial result is

$$Q_{100}(\beta)^6 - 3Q_{100}(2\beta)Q_{100}(\beta)^4 + 3Q_{100}(2\beta)^2Q_{100}(\beta)^2 - Q_{100}(2\beta)^3. \tag{25}$$

While this is the full result of the calculation, some terms will vanish in the expressions for the virial coefficients Δb_n as they do not match the volume scaling. One can in practice ignore the volume up to this point with the knowledge that terms should not depend on the volume, but for precision and clarity, the source of volume as demonstrated in calculating Q_{111} comes from the sums in position. In the full expression for the virial coefficients, powers of Q_{100} will actually cancel, however one can quickly see that the only surviving term will be

$$\frac{-Q_{100}[2\beta]^3}{3Q_{100}} \tag{26}$$

4 FORM code

As visibile in the previous calculation, things will get out of hand very quickly, even for such small systems. Initial attempts to do the determinants naively in Mathematica required complex syntax, long run times, and led to memory issues. While initial progress with the Mathematica code was inspiring, using FORM at the suggestion of Dr. Joaquín Drut led to the successful calculation of higher order terms. FORM is a symbolic algebra software designed for high-energy physics calculations. Fig.1 compares the code to other popular software.

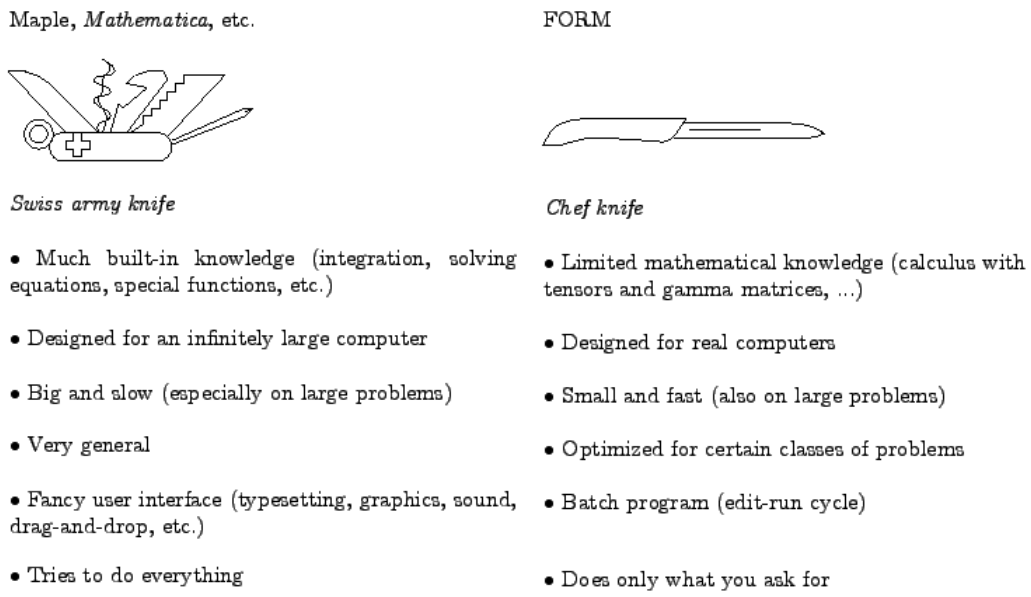

Figure 1: Comparison of software (2)

The advantage of using FORM is that the code is quite concise and efficient, without the guidance that Mathematica needs to calculate similar quantities. For a rough comparison, calculating Q_{611} took approximately two minutes on a modest (made in 2010) laptop using FORM, while on a similar system, the Mathematica code spend over thirty minutes.

The simplicity of the FORM code makes it possible to automate the code writing process. A python script was used that could first generate code, then execute all the newly made files, and finally call another script that processes the output. Unfortunately, the number of output terms quickly becomes unwieldy, so we the script that processes the output using graph theory libraries became rather complex, which will be described in the next section. It is possible to quickly process the results by hand, but having already been spoiled by the automation thus far, it was an obvious aesthetic requirement to continue the process.

Since we have an idea for the output of our calculations, we can use some shortcuts. For evaluating the determinants we begin with the Levi-Civita form

$$\det A = \epsilon_{i_1 \ldots i_n} a_{1 i_1} \ldots a_{n i_n}. \tag{27}$$

Since we square the determinant, we have two epsilon tensors for each flavor, for a total of 6 epsilon tensors. Since we know that inevitably summing of x_n will give us delta functions, we can skip right to this in writing the code. Ultimately the arguments of the delta functions are the momentum variables for fermions of each flavor.

4.1 Two-Body Example

A thorough and somewhat familiar example is the case for calculating ΔQ_{33} for a system with two-body forces and two flavors of fermions (spin up and spin down). Using i, j, k, l as indices and p, q as the momentum variables for spin up and down, we begin with the full form of the input, which is

$$\epsilon_{i_1 i_2 i_3} \epsilon_{j_1 j_2 j_3} \epsilon_{k_1 k_2 k_3} \epsilon_{l_1 l_2 l_3} \delta(p_{i_1} - p_{j_1}) \delta(p_{i_2} - p_{j_2}) \delta(p_{i_3} - p_{j_3}) \delta(q_{k_1} - q_{l_1}) \delta(q_{k_2} - q_{l_2}) \delta(q_{k_3} - q_{l_3}). \tag{28}$$

For shorthand, $\epsilon_{i_1 i_2 i_3} = \epsilon_i$, even though the tensor is of order 3. For each order in C, that is, the number of simultaneous interactions that are occurring, we contract two delta functions of opposite flavor. For order C we have

$$\epsilon_i \epsilon_j \epsilon_k \epsilon_l \delta(p_{i_1} - p_{j_1} + q_{k_2} - q_{l_2}) \delta(p_{i_2} - p_{j_2}) \delta(p_{i_3} - p_{j_3}) \delta(q_{k_1} - q_{l_1}) \delta(q_{k_3} - q_{l_3}). \tag{29}$$

This corresponds to the diagram.

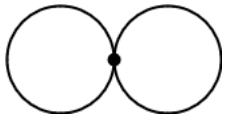

Figure 2: The first-order vacuum bubble diagram for 2-body interactions

Order C^2 is

$$\epsilon_i\epsilon_j\epsilon_k\epsilon_l\delta(p_{i_1}-p_{j_1}+q_{k_2}-q_{l_2})\delta(p_{i_2}-p_{j_2}+q_{k_1}-q_{l_1})\delta(p_{i_3}-p_{j_3})\delta(q_{k_3}-q_{l_3}). \quad (30)$$

The diagrams here are

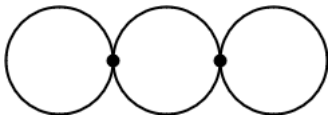

Figure 3: A second order two-body diagram, this would be where there is one four-term delta and two two-term deltas surviving

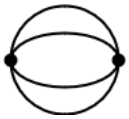

Figure 4: Another of the two second order two-body diagram, this one for two four-term deltas

At order C^3, we are evaluating three interactions, the expression of which takes the form

$$\epsilon_i\epsilon_j\epsilon_k\epsilon_l\delta(p_{i_1}-p_{j_1}+q_{k_2}-q_{l_2})\delta(p_{i_2}-p_{j_2}+q_{k_1}-q_{l_1})\delta(p_{i_3}-p_{j_3}+q_{k_3}-q_{l_3}). \quad (31)$$

Each of which corresponds to the third order bubble diagrams.

Figure 5: One of four third order diagrams

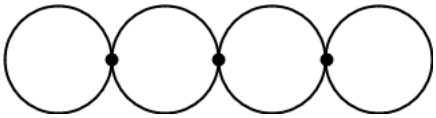

Figure 6: The second third order diagram

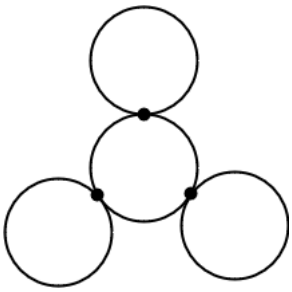

Figure 7: The third of four third order diagrams

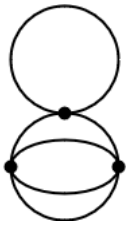

Figure 8: The last third order diagram

4.2 Three-Body Method

For three-body interactions the calculation starts with the uncontracted form, using Q_{222} again and w as the third momentum variable. Note that we now have three sets of two Levi-Civita tensors, each set of order equal to the number of particles of that flavor. Q_{222} for example will have six second order tensors, which takes the form,

$$\begin{aligned}\epsilon_i\epsilon_j\epsilon_k\epsilon_l\epsilon_m\epsilon_n\delta(p_{i_1}-p_{j_1})\delta(q_{k_1}-q_{l_1})\delta(w_{m_1}-w_{n_1})\\ \times\delta(p_{i_2}-p_{j_2})\delta(q_{k_2}-q_{l_2})\delta(w_{m_2}-w_{n_2}).\end{aligned} \tag{32}$$

Thus, we find C and C^2 by contracting one and two delta functions respectively:

$$\begin{aligned}\epsilon_i\epsilon_j\epsilon_k\epsilon_l\epsilon_m\epsilon_n\delta(p_{i_1}-p_{j_1}+q_{k_1}-q_{l_1}+w_{m_1}-w_{n_1})\\ \times\delta(p_{i_2}-p_{j_2})\delta(q_{k_2}-q_{l_2})\delta(w_{m_2}-w_{n_2}),\end{aligned} \tag{33}$$

$$\begin{aligned}\epsilon_i\epsilon_j\epsilon_k\epsilon_l\epsilon_m\epsilon_n\delta(p_{i_1}-p_{j_1}+q_{k_1}-q_{l_1}+w_{m_1}-w_{n_1})\\ \times\delta(p_{i_2}-p_{j_2}+q_{k_2}-q_{l_2}+w_{m_2}-w_{n_2}).\end{aligned} \tag{34}$$

The delta functions of six arguments may look rather strange. As a visual aid, diagrams can be helpful here, but are quite rare in the literature. For the interested reader or graph theorist, a few of the diagrams that come from the three-body interaction are below. It should be noted that no calculation is specific to one diagram, but the combinations of indices result in delta function

structures that resemble diagrams at each order. FORM is essentially computing symmetry factors to these diagrams, but we will need to use more specific software to process our output.

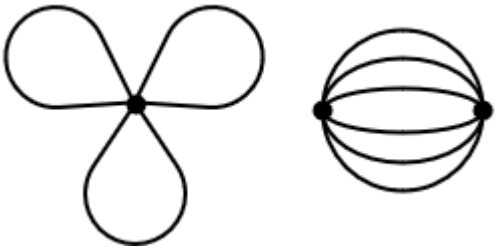

Figure 9: Sample diagrams for order 1 and 2 (there are more for order 2)

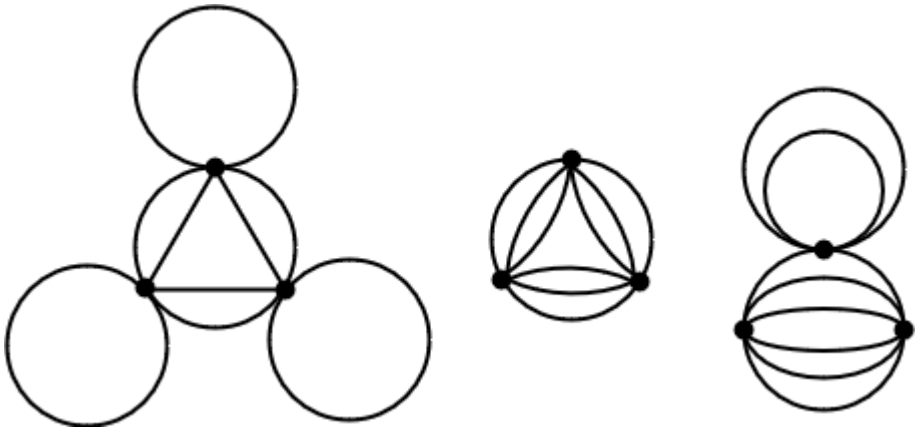

Figure 10: Sample diagrams for order 3 (there are many more) note the interesting correspondence to the two-body diagrams

5 Output Processing

The cost of using FORM is that we do lose out on some of the simplification methods in other symbolic languages. However, Mathematica even lacks methods for simplifying terms resulting from the calculation. To address this situation, a set of python codes was used using the networkx library. The group used the original code for processing the results for the two-body system. There are a number of obstacles in the way simply using the same code for three-bodies, so several significant modifications were made to handle the terms arising from contracting three delta functions in the epsilon tensor formula. The original code, written by Yaqi Hou and Dr. Joaquín Drut was modified successfully to process this data.

There are three main phases to the code

- Use the graph theory library networkx to simplify the initial terms
- Act these terms on partition functions
- Convert result to products of single particle canonical partition functions

Somewhere between items two and three, for higher orders of C, we must deal with the interesting terms that result, like for Q_{222} at order C^2, there are the two terms

$$\begin{aligned} &3F(p_1+q_1-q_2)F(p_1)F(q_2)F(q_1)Q_{100}(\beta)Q_{100}(\beta) \\ -&F(p_1+q_1+w_1-q_2-w_1)F(p_1)F(q_2)F(q_1)F(w_1)F(w_1). \end{aligned} \tag{35}$$

Where for Fermi gasses,

$$F(p) = e^{p^2/2m} \tag{36}$$

In the final calculation for Δb_n we integrate these functions. In more detail, the code first reads in the results and removes redundant delta functions and merges identical terms by creating graphs for each delta function and checking for isomorphisms between graphs. A visual explanation follows in Figures 11, 12, and 13.

Last we have to process the more complex terms that arise at higher orders. At order C, one can write all ΔQ in terms on the 1 particle partition function Q_{100}. This is not the case at C^2 or higher. To simplify these terms, we add direction to the graphs, so that lines move always from node to pseudonode, and from positive term pseudonodes to negative term pseudonodes. Figure 14 is an example of this last type of graph.

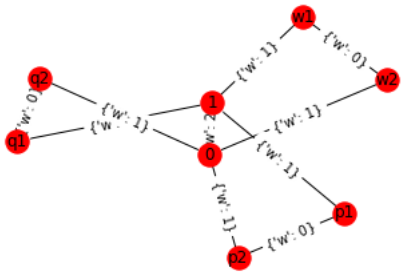

Figure 11: A six term delta graph, note the three nodes for each terms (terms with positive sign) going into the numbered node (referred to as a pseudonode) and three (negative sign terms) going into the other pseudonode. To help clarify, lines that connect nodes to nodes (2 term deltas) are given a weight of $w = 0$, nodes to pseudonodes are given a weight of $w = 1$ and pseudonode-pseudonode connections are $w = 2$

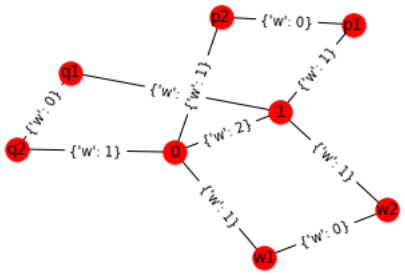

Figure 12: This graph, although with different momentum variables, gives the same final results as the figure above, so the code treats them as the same variable i.e. if $a = b, a * b = a^2$

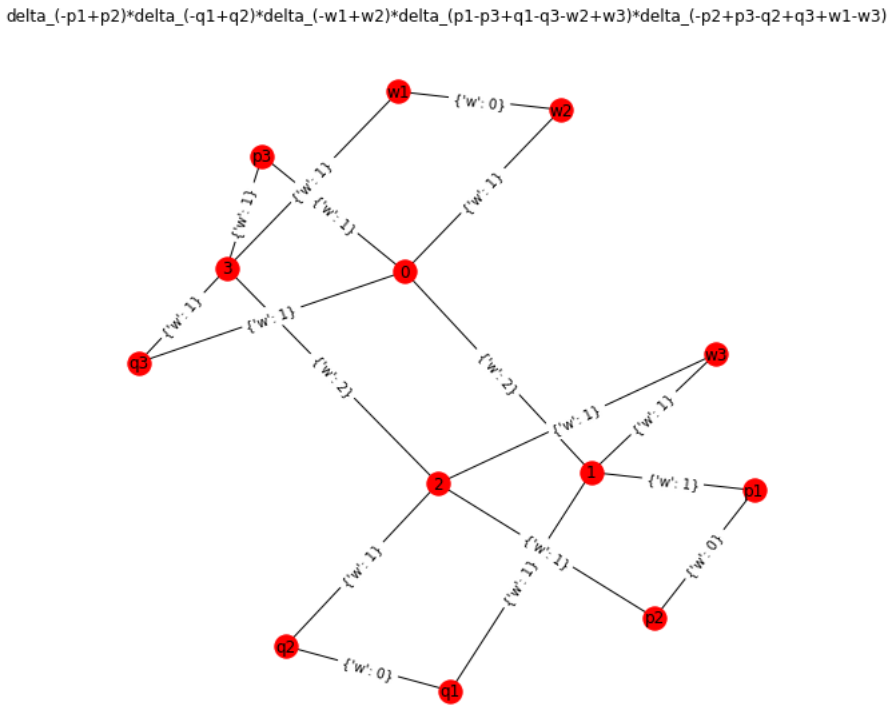

Figure 13: A more complex example, with the raw FORM code visible above. Again, each numbered pseudonode is only there to connect terms of opposite signs. While this process moves relatively quickly, a running problem in graph theory is to find faster algorithms to check for isomorphisms between graphs. This terms in one of the more complex terms, still quite feasible, but if we were interested in many-body forces of boson gasses or many-flavor many-body systems of fermions, it would be possible for this step to become quite challenging to do naively.

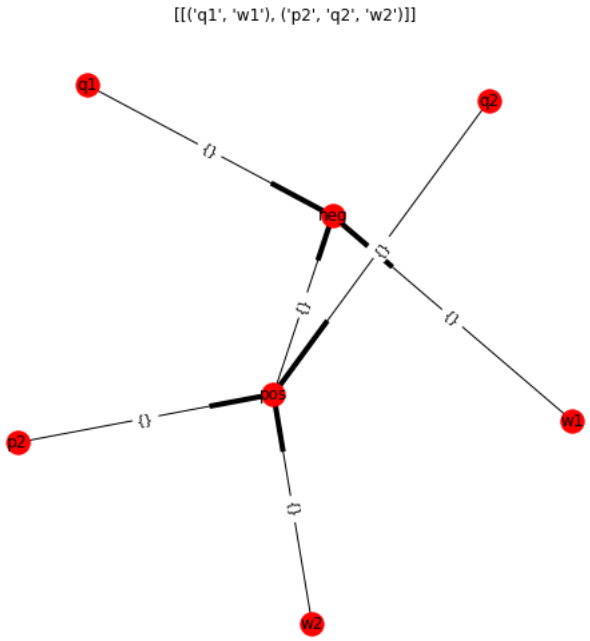

Figure 14: The directed graphs for simplifying the final simplification. In the python list describing the graph, the negative terms are first. Looking at the graph, one can see this drawn out. In the original notation of the calculation, this term would look like $e^{\beta(p_2+q_2-q_1+w_2-w_1)^2/2m}$.

6 Results

We know immediately that Δb_1 and Δb_2 are 0 since there are no three-body interactions with 1 or 2 particles. The rest require calculation using the recipes below.

$$Q_1\Delta b_3 = \Delta \mathrm{Q}_3 \tag{37}$$

$$Q_1\Delta b_4 = \Delta \mathrm{Q}_4 - \Delta \mathrm{b}_3 Q_1^2 \tag{38}$$

$$Q_1\Delta b_5 = -\, b_2\Delta \mathrm{b}_3 Q_1^2 + \Delta \mathrm{Q}_5 - \frac{1}{2}\Delta \mathrm{b}_3 Q_1^3 - \Delta \mathrm{b}_4 Q_1^2 \tag{39}$$

$$Q_1\Delta b_6 = -\, b_3\Delta \mathrm{b}_3 Q_1^2 - b_2 Q_1^2\left(\Delta \mathrm{b}_4 + \Delta \mathrm{b}_3 Q_1\right) + \Delta \mathrm{Q}_6 - \tag{40}$$

$$\frac{1}{2}\Delta \mathrm{b}_3 Q_1^4 - \frac{1}{2}\Delta \mathrm{b}_4 Q_1^3 - \Delta \mathrm{b}_5 Q_1^2 \tag{41}$$

$$Q_1\Delta b_7 = -\,\frac{1}{2}b_2\Delta \mathrm{b}_3 Q_1^4 - \frac{1}{2}b_2^2\Delta \mathrm{b}_3 Q_1^3 - b_3\Delta \mathrm{b}_3 Q_1^3 - b_2\Delta \mathrm{b}_4 Q_1^3 - \tag{42}$$

$$b_4\Delta \mathrm{b}_3 Q_1^2 - b_3\Delta \mathrm{b}_4 Q_1^2 - b_2\Delta \mathrm{b}_5 Q_1^2 + \Delta \mathrm{Q}_7 - \tag{43}$$

$$\frac{1}{8}\Delta \mathrm{b}_3 Q_1^5 - \frac{1}{2}\Delta \mathrm{b}_4 Q_1^4 - \frac{1}{2}\Delta \mathrm{b}_5 Q_1^3 - \Delta \mathrm{b}_6 Q_1^2 \tag{44}$$

$$Q_1\Delta b_8 = -\,\frac{1}{2}b_2\Delta \mathrm{b}_3 Q_1^5 - \frac{1}{2}b_2^2\Delta \mathrm{b}_3 Q_1^4 - \frac{1}{2}b_3\Delta \mathrm{b}_3 Q_1^4 - \frac{1}{2}b_2\Delta \mathrm{b}_4 Q_1^4 - \tag{45}$$

$$b_2 b_3\Delta \mathrm{b}_3 Q_1^3 - b_4\Delta \mathrm{b}_3 Q_1^3 - \frac{1}{2}b_2^2\Delta \mathrm{b}_4 Q_1^3 - b_3\Delta \mathrm{b}_4 Q_1^3 - \tag{46}$$

$$b_2\Delta \mathrm{b}_5 Q_1^3 - b_5\Delta \mathrm{b}_3 Q_1^2 - b_4\Delta \mathrm{b}_4 Q_1^2 - b_3\Delta \mathrm{b}_5 Q_1^2 - b_2\Delta \mathrm{b}_6 Q_1^2 + \tag{47}$$

$$\Delta \mathrm{Q}_8 - \frac{1}{8}\Delta \mathrm{b}_3 Q_1^6 - \frac{1}{8}\Delta \mathrm{b}_4 Q_1^5 - \frac{1}{2}\Delta \mathrm{b}_5 Q_1^4 - \frac{1}{2}\Delta \mathrm{b}_6 Q_1^3 - \Delta \mathrm{b}_7 Q_1^2 \tag{48}$$

The systematic cancellation of powers of Q_1 are slightly more obvious now. We now must insert the forms of three-body partition functions from Section 2.2. The full expressions become too large to large to print at higher orders. Data also exists for Δb_9, but only the results up to order 5 will be discussed. The remainder will be included in an upcoming publication by the group, as they still require sophisticated analysis methods to process the large outputs.

It is worth noting that the terms simplified by the directed graphs, appearing earlier as functions F, can be evaluated using the process

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}P^T M P} d^n p = \sqrt{\det 2\pi M^{-1}} \tag{49}$$

Where P is a vector of the momentum variables, and M is a symmetric matrix characterizing the equations in the F functions in n dimensions.

Additionally, in the remaining resulting partition function, the Gaussian integrals can be quickly performed to get results in any dimension using the equation

$$Q_{100}(n\beta) = \int_{-\infty}^{\infty} e^{-n\beta p^2/2m} d^D p \tag{50}$$

Which becomes in D dimensions

$$\left(\frac{2\pi}{\beta mn}\right)^{D/2} \tag{51}$$

6.1 ΔQ_{LMN}

Using the ΔQ values calculated from an initial approximation, by performing dimensional analysis and removing all terms that do not scale like the volume squared, as present in Δb_3, the following are obtained. These are likely only valid as first order approximation in C as they agree with the groups calculation for up to Δb_5, this will be investigated in the upcoming paper.

$$\Delta Q_{111} = C\frac{Q_{100}(\beta)^2}{3V^2} \tag{52}$$

$$\Delta Q_{211} = -C\frac{Q_{100}(\beta)Q_{100}(2\beta)}{6V^2} \tag{53}$$

$$\begin{aligned} \Delta Q_{311} &= C\frac{Q_{100}(\beta)Q_{100}(3\beta)}{9V^2} \\ \Delta Q_{221} &= C\frac{Q_{100}(2\beta)^2}{12V^2} \end{aligned} \tag{54}$$

$$\begin{aligned} \Delta Q_{411} &= -C\frac{Q_{100}(\beta)Q_{100}(4\beta)}{12V^2} \\ \Delta Q_{321} &= -C\frac{Q_{100}(2\beta)Q_{100}(3\beta)}{18V^2} \\ \Delta Q_{222} &= -C\frac{Q_{100}(2\beta)^3}{24V^2Q_{100}(\beta)} \end{aligned} \tag{55}$$

$$\begin{aligned} \Delta Q_{511} &= C\frac{Q_{100}(\beta)Q_{100}(5\beta)}{15V^2} \\ \Delta Q_{421} &= C\frac{Q_{100}(2\beta)Q_{100}(4\beta)}{24V^2} \\ \Delta Q_{322} &= C\frac{Q_{100}(2\beta)^2Q_{100}(3\beta)}{36V^2Q_{100}(\beta)} \end{aligned} \tag{56}$$

$$\begin{aligned}
\Delta Q_{611} &= -C\frac{Q_{100}(\beta)Q_{100}(6\beta)}{18V^2} \\
\Delta Q_{521} &= -C\frac{Q_{100}(2\beta)Q_{100}(5\beta)}{30V^2} \\
\Delta Q_{431} &= -C\frac{Q_{100}(3\beta)Q_{100}(4\beta)}{36V^2} \\
\Delta Q_{422} &= C\frac{Q_{100}(2\beta)^2Q_{100}(4\beta)}{48V^2Q_{100}(\beta)} \\
\Delta Q_{332} &= -C\frac{Q_{100}(2\beta)Q_{100}(3\beta)^2}{54V^2Q_{100}(\beta)}
\end{aligned} \tag{57}$$

From the above we can find the general form of this approximation for ΔQ_{LMN} including the final division by Q_1 as

$$(-1)^{L+M+N+1}C\frac{Q_{100}(L\beta)Q_{100}(M\beta)Q_{100}(N\beta)}{3LMNQ_{100}(\beta)V^2} \tag{58}$$

6.2 Δb_N in 1D

As mentioned earlier, up to Δb_5 have been confirmed with other calculations in the group for 1D (the dimension-general form will be given shortly). Δb_3 is used as a renormalizing parameter for ease of analysis. It is worth noting that while the analysis is consistent to Δb_5 it is possible it diverges afterward. This will be the subject of the upcoming paper, and will be investigated using more sophisticated methods, namely, automating the integration process for the $n\beta$ partition functions using the matrix form in eq.49. In 1D, where $\hbar = m = k_B = 1$, and using the dimensional approximation, the virial coefficients in 1D are

$$\Delta b_1 = 0 \tag{59}$$

$$\Delta b_2 = 0 \tag{60}$$

$$\Delta b_3 = C\left[\frac{2\pi}{3\beta}\right] \tag{61}$$

$$\Delta b_4 = -\frac{3\Delta \mathrm{b}_3}{2\sqrt{2}} \tag{62}$$

$$\Delta b_5 = \frac{3}{2}\left(\frac{1}{4} + \frac{2}{3\sqrt{3}}\right)\Delta \mathrm{b}_3 \tag{63}$$

$$\Delta b_6 = \frac{3}{2}\left(-\frac{1}{4} - \frac{\sqrt{\frac{2}{3}}}{3} - \frac{1}{24\sqrt{2}}\right)\Delta \mathrm{b}_3 - \frac{27}{16}\left(\sqrt{2}-1\right)\Delta \mathrm{b}_3^2 \tag{64}$$

$$\begin{aligned}
\Delta b_7 = \frac{1}{224}\left(168 - 21\sqrt{2} + 56\sqrt{3} - 48\sqrt{7}\right)\Delta \mathrm{b}_3^2 + \\
\frac{3}{2}\left(\frac{1}{4\sqrt{2}} + \frac{1}{12\sqrt{3}} + \frac{2}{5\sqrt{5}}\right)\Delta \mathrm{b}_3
\end{aligned} \tag{65}$$

$$\Delta b_8 = \frac{9}{4}\left(\frac{1}{189}\left(-21\sqrt{2}+7\sqrt{3}-14\sqrt{6}+3\sqrt{14}\right)+\right.$$
$$\left.\frac{336\sqrt{10}+120\sqrt{14}-35\left(33+33\sqrt{2}-8\sqrt{3}+16\sqrt{6}\right)}{10080}\right)\Delta \mathrm{b}_3^2+ \tag{66}$$
$$\frac{3}{2}\left(-\frac{1}{32}-\frac{\sqrt{\frac{2}{5}}}{5}-\frac{1}{27\sqrt{2}}-\frac{1}{6\sqrt{3}}-\frac{1}{3\sqrt{6}}\right)\Delta \mathrm{b}_3$$

The dimension-general results, as confirmed by the group are

$$\Delta b_4 = -\frac{3}{2}\frac{Q_{100}(2\beta)}{Q_{100}}\Delta b_3 = -\frac{3}{2^{d/2+1}}\Delta b_3 \tag{67}$$

$$\Delta b_5 = \left[\frac{3Q_{100}^2(2\beta)}{Q_{100}}+\frac{Q_{100}(3\beta)}{Q_{100}}\right]\Delta b_3 = \left[\frac{3}{2^d}+\frac{1}{3^{d/2}}\right]\Delta b_3 \tag{68}$$

Which agree with the 1D results above.

6.3 Plots

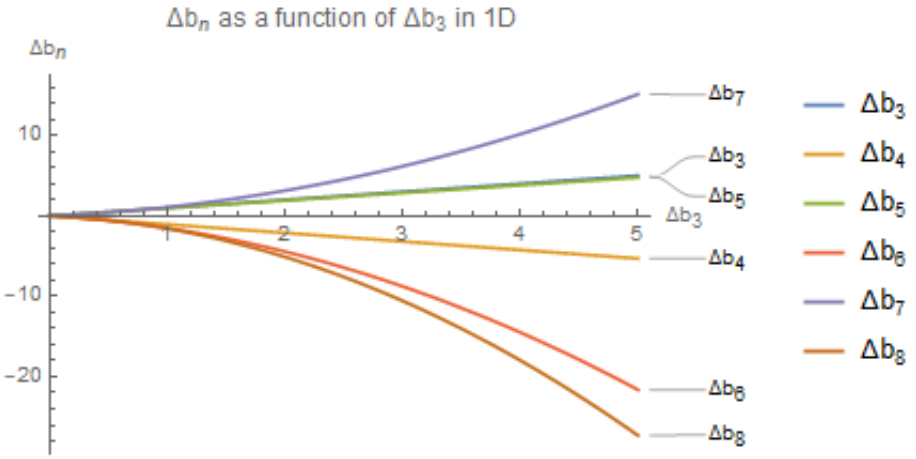

Figure 15: The virial coefficients as a function of Δb_3

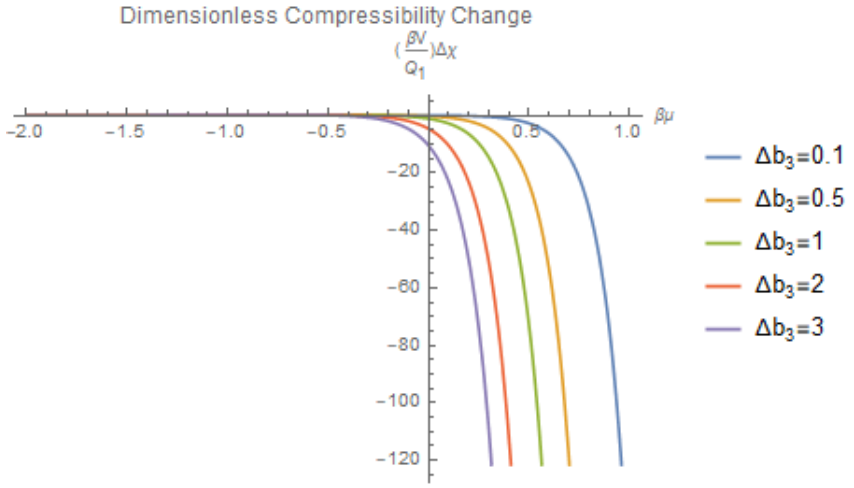

Figure 16: The (dimensionless) compressibility change as a function of $\beta\mu$ at several Δb_3

References

[1] E. Epelbaum, A. Nogga, W. Glöckle, H. Kamada, Ulf-G. Meißner, and H. Witała. Three-nucleon forces from chiral effective field theory. *Phys. Rev. C*, 66:064001, Dec 2002.

[2] André Heck. Form for pedestrians, Oct 2000.

[3] Maksim Kunitski, Stefan Zeller, Jörg Voigtsberger, Anton Kalinin, Lothar Ph. H. Schmidt, Markus Schöffler, Achim Czasch, Wieland Schöllkopf, Robert E. Grisenti, Till Jahnke, Dörte Blume, and Reinhard Dörner. Observation of the efimov state of the helium trimer. *Science*, 348(6234):551–555, 2015.

[4] B. A. Loiseau and Y. Nogami. Three-nucleon force. *Nuclear Physics B*, 2:470–478, August 1967.

[5] P. Mermod, J. Blomgren, B. Bergenwall, A. Hildebrand, C. Johansson, J. Klug, L. Nilsson, N. Olsson, M. Österlund, S. Pomp, U. Tippawan, O. Jonsson, A. Prokofiev, P.-U. Renberg, P. Nadel-Turonski, Y. Maeda, H. Sakai, and A. Tamii. Search for three-body force effects in neutron–deuteron scattering at 95 mev. *Physics Letters B*, 597(3):243 – 248, 2004.

[6] Scott E. Pollack, Daniel Dries, and Randall G. Hulet. Universality in three- and four-body bound states of ultracold atoms. *Science*, 326(5960):1683–1685, 2009.

[7] A. J. Sarty. *a Measurement of the Three-Body Photodisintegration of HELIUM-3 and its Relation to Three-Body Forces.* PhD thesis, THE UNIVERSITY OF SASKATCHEWAN (CANADA)., 1993.

[8] C. R. Shill and J. E. Drut. Virial coefficients of one-dimensional and two-dimensional fermi gases by stochastic methods and a semiclassical lattice approximation. *Phys. Rev. A*, 98:053615, Nov 2018.

[9] Masuo Suzuki. Generalized trotter's formula and systematic approximants of exponential operators and inner derivations with applications to many-body problems. *Communications in Mathematical Physics*, 51(2):183–190, Jun 1976.