

# Determining an Effective Theory Interaction for a Quantum Gas in the Unitary Limit

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My main project was to solve a problem that would describe the interaction of a two particle system of a quantum gas in the unitary limit. When interacting, gases of particles in the unitary limit have a single bound state of zero energy in free space. My project was to determine the interaction that could be used to describe the case of a system of two such particles for an effective reduced basis set of harmonic oscillator eigenstates of arbitrary size. The problem in the unitary limit would be useful for solving problems for particles in high potentials that are very weakly bound. Before my main project, I learned the basic idea of what an effective theory is. An effective theory is a low energy model for a potential energy involving high energy physics that we can't see. A wave function cannot be sensitive to a potential that acts over a width much smaller than its wavelength, so the low energy solutions to the Schrodinger equation for a given potential whose wave functions are very broad compared to the range at which the details of the potential operate will not be very much affected and therefore we can find accurate solutions to the problem in perturbation theory. If we don't know exactly what the potential looks like, we can treat the unknown short range potential as a perturbation of the long range potential with parameters to be fit to agree exactly with the lowest energy measurements. Then we can apply these parameters to higher energies to provide a good approximation within a certain energy range.

In first order perturbation theory, the energy shift from the perturbing potential  $V(r)$  is given by  $\int |\Psi(r)|^2 V(r) d^3r$ . If the unperturbed energy is smooth, we can expand the wave function in a Taylor series around the origin where the integral becomes

$$\int \left( |\Psi(r)|^2 V(r) \Big|_{r=0} + r \frac{d}{dr} |\Psi(r)|^2 \Big|_{r=0} V(r) + \frac{1}{2} r^2 \frac{d^2}{dr^2} |\Psi(r)|^2 \Big|_{r=0} V(r) + \dots \right) d^3r \quad (1)$$

which means that the perturbing potential within the integral over the position space essentially acts like a linear combination of a delta function and its derivatives, ie, picking out the values of the successive derivatives at the origin, each one weighted by a strength determined by the evaluation of each integral this action is multiplied by. Following the idea that the true perturbing potential acts like an infinite linear combination of delta function derivatives, in our effective theory we can approximate the perturbing potential as such, but only keep a finite number of terms. We do not know the potential so we do not know the constants in front of the delta function, but if we decide to only include a finite number of terms we can determine an approximation to them by requiring that they are consistent with the low energy measurements.

A simple example that I explored to illustrate this point was an infinite square well with a small square well cut out of it in the middle. We knew the unperturbed potential (infinite square well) with energies  $E_N^{(0)}$  and wave function  $\Psi_N^{(0)}$ . Suppose I wanted to use  $m$  terms. Then I would approximate the energy shift from the perturbing potential by

$$E_N^{(1)} = \sum_{n=0}^m a_n \frac{d^n}{dr^n} |\Psi(r)|_{r=0} .$$

Then one would choose coefficients so that the correction for the lowest energy produces the exact experimental results for  $E_1$  up to  $E_m$ . For example in the case of the perturbed well, we use the first two nonzero terms  $a_0$  and  $a_2$ . One would demand  $E_2 - E_2^{(0)} = a_0 |\Psi_2^{(0)}(r)|^2|_{r=0} + a_2 \frac{d^2}{dr^2} |\Psi_2^{(0)}(r)|_{r=0}$  and  $E_1 - E_1^{(0)} = a_0 |\Psi_1^{(0)}(r)|^2|_{r=0} + a_2 \frac{d^2}{dr^2} |\Psi_1^{(0)}(r)|^2|_{r=0}$ . Then one would solve for  $a_0$  and  $a_2$  and apply the resulting potential to determine the energy corrections for all higher states. As a result, one would find that as more terms are added, the error between the true energy and the energy given by first order perturbation theory decreases for the higher states within a certain range. At significantly higher energies, the wave function becomes more oscillatory and the higher order terms in the expansion become more important. Eventually, the answer starts off very inaccurate and one does not converge on the right answer no matter how many more correction terms are added. In other words, the situation is non-perturbative. The wave function can probe the details of the potential which make a difference in its structure; treating the details as a perturbation is not adequate to describe the solutions.

After I understood the idea of an effective theory, I moved on to my main project. I worked on a problem that would be useful for people dealing with situations in nuclear physics that involve particles in high potentials which are very weakly bound. My problem dealt with the case of a quantum gas in the unitary limit, in which two particles interact through a sharp potential and have a single bound state of zero energy in free space. Eventually the aim was to solve the eigenvalue problem for the particles in a harmonic trap. This problem would be most naturally solved in the basis of harmonic oscillator eigenstates. But we cannot use all the states. This is where the idea of an effective theory comes in: we must find an expression for the parameter of the potential that gives a unitary quantum gas for an arbitrary cutoff number of states in that basis. Therefore, I had to substitute the Hamiltonian for a unitary gas in free space into the eigenvalue problem setting  $E=0$  for an arbitrarily sized reduced basis of harmonic oscillator eigenstates and solve for  $a$  to determine its dependence on the basis. The value of  $a$  giving approximate the interaction, up to a certain scale which we defined, as being a fuzzy delta function. More specifically, we defined the interaction by:

$$\langle N' | a\delta(r) | N \rangle = a\Psi_{N'}(r)\Psi_N(r) |_{r=0}, \quad (2)$$

if  $N'$  and  $N$  are less than or equal to  $\Lambda$ , and 0 if one of them is greater than  $\Lambda$ , where  $\Lambda$  is a cutoff wavelength. It is therefore said to be a fuzzy delta function because it only operates between basis eigenstates up to a certain scale. We cannot use a true delta function, the particles would not interact at all because to do so they would have to occupy the same exact point in space which is impossible. Using a delta function means that contribution to the potential energy's action on the matrix elements  $\langle N', l, m | H | N, l, m \rangle$  is zero for all but the matrix elements within our range of  $N=0$  to  $\Lambda$  in which the Hamiltonian is between  $s$  states, ie,  $l$  and  $m$  are both zero. This is because a delta function takes the product of the product of the bra and ket wavefunction at the origin, and only  $s$  waves have a nonzero value at the origin. If one set up the complete Hamiltonian for the eigenvalue problem that sets  $E=0$ , grouping the states together by values of angular momentum, and looked at the resulting matrix, one would also find that the kinetic energy operator only produces a nonzero value for a given matrix element when acting between two states which have the same angular momentum. This is because the angular dependence of the states is expressed by a single spherical harmonic, and hence is an eigenstate of the kinetic energy operator, so the matrix elements will be nonzero only if the two spherical harmonics

are the same, and for this to occur the angular momentum must be the same. So if we look at the Hamiltonian for Hunitary, we see that there is only an interaction between states that have the same angular momentum. The Hamiltonian can be expressed as  $\hat{H}_s + \hat{H}_p + \hat{H}_d +$  where  $\hat{H}_s$  produces a 0 matrix element when not acting between two s states, and likewise for the other values of angular momentum. Therefore we must have

$$\hat{H}_s | \Psi_s \rangle = E | \Psi_s \rangle$$

$$\hat{H}_p | \Psi_p \rangle = E | \Psi_p \rangle$$

where  $|\Psi\rangle = |\Psi_s\rangle + |\Psi_p\rangle + |\Psi_d\rangle +$  and the eigenvalues and eigenstates are determined that way as being states made up of linear combinations of states of the same angular momentum. The form of this matrix is advantageous because it means that all we have to do to determine the a giving  $E=0$  is to solve  $\hat{H}_s | \Psi_s \rangle = 0$ . S states have  $m=0$ , so we can label them uniquely by their principle quantum number,  $N$ , where  $E = \left(N + \frac{3}{2}\right) \hbar\omega$ . From the form of the solution to the eigenvalue problem,  $N = 2n_r + l$ , where  $n_r$  is the number of nodes in the radial wave function. Since we are only using s states,  $l=0$  for all states, and  $N$  is an even integer. Our basis includes states  $N=0$  up to  $N = \Lambda$ , the cutoff value of  $N$  in our basis. Once I solved this problem and obtained the interaction that accommodates a certain choice of basis., I could put the particles in a harmonic trap, the problem could be more easily solved. The matrix would be diagonal everywhere except for where the Hamiltonian acts between two s states, and we would just have to diagonalize this part of the Hamiltonian. We must account for the fact that it is not true that if we include the wavefunction as a linear combination of a high number of basis harmonic oscillator eigenfunctions that we will converge on the right answer for the wave function of this gas. This is because the wavefunction of a particle that is just barely bound is able to extend all the way out of the potential well. The higher the energy of the states we include in the linear combination, the broader the wavefunction, but after a certain point, each wavefunction dies off exponentially. Also, the actual wavefunction builds up more and more inside the well. The higher the energy states we use, the higher the corrections are needed. The unitary limit is an a limiting case of very small binding energy, and we cannot converge on the right answer to this problem no matter how many states we include in the basis. However, there is a way to get the exact answer

in which we use the Bloch-Horowitz equation: This equation gives the effective Hamiltonian that we must use in order to get the same value for the energy that we would get with the true Hamiltonian. The Bloch-Horowitz equation is given by:  $\hat{P} \left( \hat{H} + \hat{H} \hat{Q} \frac{1}{E - \hat{Q} \hat{H}} \hat{Q} \hat{H} \right) \hat{P} | \Psi \rangle = E \hat{P} | \Psi \rangle$ . Where  $\hat{P}$  is the projection of the complete basis onto the space, and  $\hat{Q}$  is the projection of the complete basis that lies outside the space. So instead of applying the operator  $\hat{H}$  between each of the matrix elements from our reduced basis, we apply the effective Hamiltonian  $\hat{H}_{eff} = \hat{H} + \hat{H} \hat{Q} \frac{1}{E - \hat{Q} \hat{H}} \hat{Q} \hat{H}$ . The uncorrected matrix elements  $\langle i | \hat{H} | j \rangle$  of the free space Hamiltonian for a unitary gas is given by  $\langle i | \frac{\hbar^2}{2m} \nabla^2 + a_\Lambda \delta(r) | j \rangle$ . We will correct for the fact that we only use a reduced basis using the correction  $\hat{H} \hat{Q} \frac{1}{E - \hat{Q} \hat{H}} \hat{Q} \hat{H}$ . It can be shown that applying the kinetic energy operator to a state  $| N \rangle$  we obtain  $-\frac{\hbar^2}{2m} \nabla^2 | N \rangle = -\frac{\hbar\omega}{2} \left( \sqrt{\frac{N}{2} \left( \frac{N+1}{2} \right)} | N - 2 \rangle + \left( N + \frac{3}{2} \right) | N \rangle + \sqrt{\left( \frac{N}{2} + 1 \right) \left( \frac{N}{2} + \frac{3}{2} \right)} | N + 2 \rangle \right)$  The kinetic energy operator therefore only takes a ket outside the space if  $N = \Lambda$ . Looking at the Bloch-Horowitz correction, we can see that the correction becomes zero unless both  $i$  and  $j$  equal  $\Lambda$ . The correction to the top matrix element can be shown to equal  $\frac{\hbar\omega}{2} \left( \frac{N}{2} + 1 \right)$ . My advisor showed this result in an earlier paper; it was not straightforward to evaluate and I did not have time to learn how to do it myself. Using this top corner matrix correction, I found the form of the Hamiltonian matrix elements for the eigenvalue problem and set the determinant equal to zero to find  $a_\Lambda$ . Although the matrix could be arbitrarily large, it could be manipulated by adding multiples of rows or columns to other rows or columns to get it into a simplified form for which the determinant could be more easily evaluated. The result was  $a_\Lambda = \frac{1}{\sum_{j=0}^{j=\lfloor \frac{\Lambda}{4} \rfloor} \frac{\Gamma(\frac{\Lambda}{2} - 2j + \frac{1}{2})}{(\frac{\Lambda}{2} - 2j)!}}$  where  $\lfloor \frac{\Lambda}{4} \rfloor$  is the greatest integer less than or equal to  $\frac{\Lambda}{4}$ . Once I solved this problem, obtaining the interaction that accommodates a certain choice of basis, if one the problem of putting the particles in a harmonic trap could be much more easily solved. The matrix would be diagonal everywhere except for where the Hamiltonian acts between two states, and we would just have to diagonalize this part of the Hamiltonian. In addition, no Bloch-Horowitz correction would be needed because the operator  $-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega \hat{r}^2 + a \delta(r)$  does not take one outside the space. The next step would be to find the relationship between  $a_\Lambda$  and  $a_{\Lambda-2}$ . This could be done by treating the effective Hamiltonian  $\hat{H}_\Lambda$  using states 0 through  $\Lambda$

as the true Hamiltonian and finding the effective Hamiltonian for a matrix that uses states 0 through  $\Lambda - 2$ . In this case,  $\hat{P} = \sum_{N=0}^{N=\Lambda-1} |N\rangle\langle N|$  and  $\hat{Q} = . | \Lambda\rangle\langle N | .$  We break up the correction to the Hamiltonian into two parts: one which we call the correction to the kinetic energy part of the Hamiltonian and one which we call the correction to the delta function part of the Hamiltonian. In the old basis the new top corner element was  $\langle \Lambda - 2 | \hat{T}_\Lambda | \Lambda - 2 \rangle$ ; now a correction of  $\langle \Lambda - 2 | \hat{T}_\Lambda | \Lambda - 2 \rangle$  is added. We can then write the correction to the delta function as what remains from the total corrected Hamiltonian if we subtract the corrected kinetic energy. I confirmed that if we use the corrected term for  $\langle \Lambda | \hat{T}_\Lambda | \Lambda \rangle$  given by subtracting  $\left(\frac{\Lambda}{2} + 1\right) \frac{\hbar\omega}{2}$ , the correction to the kinetic energy for the new top corner matrix element is given by subtracting  $\frac{\hbar\omega}{2} \left(\frac{\Lambda}{2}\right)$ , which is consistent with the requirement that the correction to any top corner matrix element is given by subtracting the value for  $\frac{\hbar\omega}{2} \left(\frac{\Lambda}{2} + 1\right)$  of that basis. Since no matter what the size of the basis we always use a delta function with coefficient  $a(\Lambda)$ , the result for the correction to the delta function would relate  $a_{\Lambda-1}$  to  $a_\Lambda$ . I am still working on the result of this relation.