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**Effective Hamiltonian Approach to Two-Atom Molecules:
Demonstration of the Method**

or

How I Spent My Summer (see the last page!)

Alex Mints

Research Experience for Undergraduates Program

Physics Department, The Ohio State University, Columbus OH 43210, USA

“It seems very pretty,’ she said when she had finished it, ‘but it’s rather hard to understand!’ (You see, she didn’t like to confess, even to herself, that she couldn’t make it out at all.) ‘Somehow it seems to fill my head with ideas – only I don’t exactly know what they are!’”

ALICE, AFTER READING “JABBERWOCKY” IN LEWIS CARROLL’S *Through the Looking-Glass and What Alice Found There*

“Physics is like sex: sure, it may give some practical results, but that’s not why we do it.”

RICHARD FEYNMAN

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I. INTRODUCTION

It is generally the case that different physics communities do not interact very much with each other. Even if physicists read papers written about physics areas other than their own, they are often not abreast of all the happenings in different specialties. Sometimes an idea with wide-ranging applications extensively used in one area is relatively obscure or even totally unknown in another. This means that in some cases physicists are missing out on new developments that, aside from being simply interesting, would actually aid in their own work.

One such development is the idea of *effective field theories* [1–3] (EFT). This very versatile tool, which has been applied extensively in high-energy and nuclear physics, is readily adaptable to atomic and molecular physics. It is a powerful technique for predicting low-energy observables when the details of the short-distance (high-momentum) interactions are unknown, as is usually the case. It allows systematic computation of these observables to theoretically any accuracy, in stark contrast to the present-day inability to get past beyond a certain (poor) accuracy in their calculations and a lack of systematic techniques.

With the upsurge of interest in Bose-Einstein condensation (see Ref. [5–7]), activity in low-energy atomic and molecular physics has increased. Theoretical predictions of many observables, such as bound state energies and scattering lengths, have become more important than ever. For instance, in order to predict many properties of Bose-Einstein condensates of certain atoms, one needs to compute the scattering length of these atoms with sufficiently high accuracy. The best results for the scattering length of ^{23}Na , for example, have an error of 10% [8], which is by far not enough for precise BEC calculations.

One of the biggest roadblocks in such work is a poor understanding of the detailed structure of short-distance interactions. For example, the interatomic forces which govern molecule formation are still unknown and can only be modeled. On the contrary, the long-distance potential can be very accurately determined because at such distances the wavefunction of the molecule becomes separable into the wavefunctions of its constituent atoms. The reason is that the atomic wavefunction overlap falls off exponentially with the distance. Therefore, the long-distance potential of a two-atom molecule can be calculated with high accuracy from the wavefunctions of each atom separately.

This overlap, however, is significant at short distances. Precise determination of the short-distance behavior is difficult, thereby severely limiting the level of accuracy that can be obtained with standard methods. These usually try to model short-range interactions themselves. It is possible, though highly unlikely, that in the future these methods will allow one to obtain sufficiently high accuracy; however, that will necessarily come at a very high price of much effort and does not guarantee systematic techniques.

An alternative way to approach the problem is to use *effective hamiltonian methods* [4] (EHM). This is the method of EFT applied to atomic physics. This model-independent¹ and easy-to-implement method allows for the calculation of low-energy observables to theoretically any accuracy. The accuracy obtained is limited only by practical considerations of time and computing power. All this can be achieved with relatively little effort.

¹In the sense that it is independent of the unknown physics at short distances.

In this paper I present the work done on this project over the summer of 1999. This was done as part of the NSF-funded Research Experience for Undergraduates Program at The Ohio State University under the advising of Eric Braaten and in association with Peter Lepage of Cornell University. Theoretical background and considerations are presented first, followed by preliminary results and their discussion.

II. LOW-ENERGY EFFECTIVE THEORIES

One can describe a given non-relativistic quantum system in terms of the potential which it produces and at the same time to which it responds. Knowing this true² potential exactly allows us to calculate all the properties of this system. For instance, to get the bound states of the system one solves the Schroedinger equation for eigenvalues:

$$\left[\frac{-\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad (1)$$

It is often the case that the potential has different behavior in different regimes. In atomic physics the potential goes to zero at large distances, and its functional form at a large separation can be determined experimentally. This fixes the long-distance behavior of the potential which can be quite different from its short-distance behavior. For that reason, it is convenient to split the true potential into the corresponding pieces:

$$V^{\text{true}}(\mathbf{r}) = V_{\text{short}}^{\text{true}}(\mathbf{r}) + V_{\text{long}}^{\text{true}}(\mathbf{r}). \quad (2)$$

Frequently we do not know the true potential. In that case it is possible to construct an *effective* potential that either tries to approximate the true potential itself, i.e., its functional form, or only its effects on some observables. Then we have

$$V_{\text{effective}}(\mathbf{r}) = V_{\text{short}}(\mathbf{r}) + V_{\text{long}}(\mathbf{r}). \quad (3)$$

In general, methods that try to find a potential such that it reproduces the observable are much better than those that try to get the actual functional form of the potential itself. It is a lot harder to look for the form of the potential when you do not know the physics underlying it. In addition, the physically significant objects are the observables and not the potential itself.

A. Two for the Price of One

The idea of EHM approach is based on an observation that all low-energy observables are sensitive to precisely the same aspects of the true short-distance potential $V_{\text{short}}^{\text{true}}(\mathbf{r})$. One does *not* need to worry about the other properties of the potential as they do not influence the observables. But those aspects to which the low-energy observables are sensitive, must

²As opposed to an artificial model potential.

be dealt with carefully. In particular, if one is able to find those relevant properties such that the potential will allow for the reproduction of data for one, experimentally known, low-energy observable, A , with a certain accuracy, then you are guaranteed that it will produce data for any other unknown low-energy observable B with similar³ accuracy [1].

Note that we are not modeling the unknown and undoubtedly very complicated short-distance interactions; there's no need for that. If a given effective potential can reproduce known low-energy data, then it can be used to predict unknown data with the similar accuracy. In order to obtain higher-accuracy data for B , one only has to find a potential that will reproduce data for A with equivalently higher accuracy.

B. Systematic Expansion

Thus, we do not know nor want to know the short-distance behavior. To be sure, we cannot simply throw that away because it certainly influences low-energy observables. We must get around that. First of all, we need to limit the influence of $V_{\text{short}}^{\text{true}}(r)$; this is accomplished by introducing an ultraviolet cutoff (expressed either in terms of a momentum Λ or a distance a) which explicitly excludes short-distance dynamics from the theory. This removes from our consideration unknown and, hence, unpredictable, effects of $V_{\text{short}}^{\text{true}}(r)$. But in throwing away these effects we are also throwing away the baby with the bathwater: these effects have to somehow be accounted for when we compute our low-energy observables. The point is not that we do not want to mimic the effects of $V_{\text{short}}^{\text{true}}(r)$, but that we do not want to include them in their true form that we don't understand and can't control; we include them in a way that is controlled by us.

This is accomplished by noticing that to a low-momentum probe (with wavelength $\lambda \gg a$) the true short-distance potential (containing whatever complicated structure) looks point-like, i.e., a delta function in real space (or configuration space). So we can replace the true short-distance potential by a collection of point-like potentials with different amplitudes. This is reminiscent of the multipole expansion of electric and magnetic fields due to charge and current distributions. And indeed, the idea is the same.

It turns out, however, that the delta function is too singular to be meaningful beyond first-order in perturbation theory, implying that one cannot improve upon these first-order results using this approach. Instead of abandoning the approach we slightly modify it by replacing the singular delta function with one that complies with our earlier ultraviolet cutoff. The effect of this UV cutoff is to smear out the delta function over a volume of radius approximately $a \sim \Lambda^{-1}$. We define the smeared out delta function by

$$\delta_a^3(r) \equiv \frac{e^{-r^2/2a^2}}{(2\pi)^{3/2}a^3}. \quad (4)$$

This allows us to perform a ‘‘multipole’’ expansion of $V_{\text{short}}(r)$. This is essentially a Taylor

³See p.6 for a way to compute the accuracy of predictions of data for an unknown observable.

expansion with the one-dimensional derivative replaced by a spherically-symmetric⁴ three-dimensional one – the laplacian ∇^2 .

The short-distance potential can be broken up into two terms, the *main* piece $V_{\text{main}}(r)$ and the *tuning* piece $V_{\text{tune}}(r)$:

$$V_{\text{short}}(r) = V_{\text{main}}(r) + V_{\text{tune}}(r). \quad (5)$$

The former is called so not because it is crucial to the theory, but because the short-distance potential V_{short} is essentially that piece with a little admixture of the tuning piece. In absence of any tuning it is only the *main* piece that gives V_{short} its form.

The basic tenet of EHM is that one can use any main potential whatsoever⁵. This unexpected statement frees us to choose whatever potential we want to represent the short-distance behavior such that it will lead to good predictions of low-energy observables. In other words, we do *not* have to seek out a potential that is reasonable or even physically plausible. In essence, pick any potential for $V_{\text{main}}(r)$ and that's it.

The tuning potential plays the role of actually fitting our choice for $V_{\text{short}}(r)$ to produce the desired data. As mentioned before, it is a Taylor expansion of a three-dimensional spherically-symmetric $\delta_a^3(r)$. We introduce multiplicative coefficients c_i that we vary (tune) so that the total potential

$$V_{\text{effective}}(r) = V_{\text{short}}(r) + V_{\text{long}}(r) \quad (6)$$

$$= [V_{\text{main}}(r) + V_{\text{tune}}(r)] + V_{\text{long}}(r) \quad (7)$$

reproduce some subset of the low-energy data. The general form for the tuning piece is

$$V_{\text{tune}}(r) = \sum_{i=0}^{n<\infty} c_{i+1} a^2 \left[a^{2i} \nabla^{2i} \delta_a^3(r) \right]. \quad (8)$$

For our purposes the first two terms will suffice. Thus, the form of the tuning potential we will be using is

$$V_{\text{tune}}(r) = c_1 a^2 \frac{e^{-r^2/2a^2}}{(2\pi)^{3/2} a^3} + c_2 a^2 \left(\frac{r^2}{a^2} - 3 \right) \frac{e^{-r^2/2a^2}}{(2\pi)^{3/2} a^3}. \quad (9)$$

It is a general feature of EHM that the more parameters you tune, the greater the accuracy you get in your predictions. This allows for a *systematic* improvement of predictions simply by using more terms in the expansion of the smeared out delta function [1].

⁴This is both to simplify the situation and because the experimental data we will be using is itself spherically-symmetric.

⁵For the sake of simplicity, we limit ourselves to at least piecewise continuous spherically-symmetric ones. So, I replace all vector- \mathbf{r} with radial- r coordinates.

C. Summary of EFT philosophy

Let us summarize *effective hamiltonian theories*. Here is the method itself:

- incorporate the exact long-distance potential $V_{\text{long}}(r)$;
- select any main short-distance potential $V_{\text{main}}(r)$;
- expand $V_{\text{tune}}(r)$ up to desired order n ;
- tune the potential by adjusting the coefficients $\{c_1, \dots, c_n\}$ to reproduce data for known low-energy observable A to desired accuracy x ;
- with this resultant tuned potential compute unknown low-energy observable B to some accuracy y ;
- estimate the error bar (and thus accuracy y) of the prediction of B by computing the maximum and minimum values for B with $n + 1$ tuning parameters, where the $(n + 1)^{\text{st}}$ tuning coefficient is within some reasonable expected range. Compare with the previous calculation of B with n coefficients⁶.

Here are the features of EHM:

- do *not* need to deal with or even know the “real” complicated short-distance behavior, use a simple model of *your choosing* instead;
- known interaction information (in form of experimental data for some low-energy observable) is incorporated by adjusting the expansion coefficients;
- tuning these coefficients to reproduce data for one (known) variable gives the potential that with similar accuracy produces data for another, unknown, variable;
- can get *systematically* better approximations by including more terms in the expansion. In particular, relative errors in bound state energies scale as $|E|$ for one tuning coefficient, $|E^2|$ for two and so on:

$$|\Delta E/E| \propto |E^n|, \tag{10}$$

where n is the number of parameters [1].

⁶The question of predicting accuracy y for results for unknown variables was brought to my attention by Prof. Lemberger. The above way of doing it was suggested to me by Prof. Furnstahl.

III. FUNDAMENTAL THEORY FOR LOW-ENERGY ATOMS

In this section, we summarize the “fundamental” theory that could in principle be used to calculate the low-energy behavior of atoms if the interatomic potential were known with sufficient accuracy. We focus on the ^{23}Na atom, because there is accurate data on the energy levels of molecular states near threshold for this atom. We use atomic units throughout. Lengths are measured in units of the Bohr radius: $a_0 = \hbar/(\alpha m_e c) = 0.529 \text{ \AA}$. Energies are measured in the unit $e_0 = \alpha^2 m_e c^2 = 27.2 \text{ eV}$, which is twice the Rydberg energy. The conversion factor for changing from cm^{-1} to atomic units is $1 \text{ cm}^{-1} = 4.5563353 \times 10^{-6} e_0$. Masses are measured in units of the electron mass m_e . The mass of the ^{23}Na atom is $M = 41907.788 m_e$.

A single ^{23}Na in its electronic ground state can be described by the following dynamical variables:

- its position \mathbf{r} ,
- its electronic spin \mathbf{S} , which has quantum number $s = \frac{1}{2}$,
- its nuclear spin \mathbf{I} , which has quantum number $i = \frac{3}{2}$.

The total hyperfine spin is $\mathbf{F} = \mathbf{S} + \mathbf{I}$, and the hyperfine spin quantum number f can be 1 or 2. The hyperfine interaction splits the ground state into two states, with the $f = 1$ state being lower in energy. The hyperfine splitting is $\Delta E_{hf} = 0.27 \times 10^{-6} e_0$. The hamiltonian that describes an isolated atom labeled by index i in the absence of electromagnetic fields is

$$H_i = -\frac{1}{2M} \nabla_i^2 + \Delta E_{hf} \frac{\mathbf{S}_i \cdot \mathbf{I}_i}{2\hbar^2}. \quad (11)$$

The quantum state for two low-energy sodium atoms in the center-of-momentum frame can be specified by

- the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ of the nuclei of the atoms or, equivalently, the radial coordinate r and the orbital angular momentum quantum numbers j, m_j ,
- the Born-Oppenheimer state of the electrons, which is denoted $^1\Sigma_g$ or $^3\Sigma_u$ for those states that asymptotically approach two ground-state atoms as $r \rightarrow \infty$,
- the quantum numbers s, m_s for the total electronic spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ (s can be 0 or 1),
- the quantum numbers i, m_i for the total nuclear spin $\mathbf{I} = \mathbf{I}_1 + \mathbf{I}_2$ (i can be 0, 1, 2, or 3).

The symmetry of the electronic states together with the Pauli exclusion principle implies $s = 0$ (spin-singlet) for $^1\Sigma_g$ and $s = 1$ (spin-triplet) for $^3\Sigma_u$. The Pauli exclusion principle applied to the nuclei also implies that $j + s + i$ should be even.

The interactions between two atoms with electronic states $^1\Sigma_g$ and $^3\Sigma_u$ are characterized by the spin-singlet potential $V_0(r)$ and the spin-triplet potential $V_1(r)$, respectively. The hamiltonian for the two-body system can be written as

$$H = H_1 + H_2 + V_0(r) \left(1 - \frac{\mathbf{S}^2}{2\hbar^2}\right) + V_1(r) \frac{\mathbf{S}^2}{2\hbar^2}, \quad (12)$$

where H_i is the one-body hamiltonian (11). If the hyperfine terms in H_1 and H_2 are neglected, then s , i , and j are all good quantum numbers and the spin-singlet ($^1\Sigma_g$) and spin-triplet ($^3\Sigma_u$) systems can be treated independently. In order to demonstrate the effective hamiltonian approach, we will focus on the spin-singlet system and ignore the hyperfine interaction. This approximation breaks down near threshold when the energy is comparable in magnitude to the hyperfine splitting $\Delta E_{hf} = 0.27 \times 10^{-6} e_0$. In this case, the hyperfine coupling between the spin-singlet and spin-triplet channels must be taken into account. The molecular states we will use to tune our effective potentials have binding energies as low as $19 \times 10^{-6} e_0$. This is sufficiently large compared to the hyperfine splitting that the hyperfine interaction can be ignored in tuning the short-distance potential.

The energy levels of the molecular states in the spin-singlet potential $V_0(r)$ can be labeled by the vibrational quantum number v and the angular momentum quantum number j , and will be denoted by $E_{v,j}$. The spin-singlet potential supports 65 S-wave ($j = 0$) vibrational levels with vibrational quantum number $v = 0, \dots, 64$. Here we adhere to the convention that the highest level, i.e., least bound, be labeled with $v = 64$ and the lowest, i.e., most bound, with $v = 0$. The potential has a minimum near $r_e = 5.818 a_0$ with a depth of $D_e = 27438.4 \times 10^{-6} e_0$ [9]. According to Model I of Ref. [10], the splitting between the ground state and the first excited state is $E_{1,0} - E_{0,0} = 718.356 \times 10^{-6} e_0$. Near its minimum, the potential can be approximated by a Morse potential:

$$V_{\text{Morse}}(r) = D_e \left[\left(1 - e^{-(r-r_e)/a_e}\right)^2 - 1 \right]. \quad (13)$$

The S-wave vibrational energy levels are known analytically for this potential:

$$E_{v,0} = \hbar\omega_e \left[-\frac{1}{4x_e} + \left(v + \frac{1}{2}\right) - x_e \left(v + \frac{1}{2}\right)^2 \right], \quad (14)$$

where $\hbar\omega_e = [4D_e\hbar^2/(Ma_e^2)]^{1/2}$ and $x_e = [\hbar^2/(4D_eMa_e^2)]^{1/2}$. The value of a_e that reproduces the splitting $E_{1,0} - E_{0,0}$ is $a_e = 2.22291 a_0$. The parameters in the formula (14) for the S-wave energy levels are then $\hbar\omega_e = 728.014 \times 10^{-6} e_0$ and $x_e = 0.00663317$. The total number of S-wave vibrational energy levels supported by this Morse potential is 75, compared to 65 for the true interatomic potential.

The effective hamiltonian approach requires accurate knowledge of the behavior of the potential at long distances. At large r , the spin-singlet potential can be expressed as the sum of a dispersion term $V_C(r)$ and an exchange term $V_X(r)$. The dispersion potential is an expansion in powers of $1/r^2$ beginning at order $1/r^6$:

$$V_C(r) = - \left(\frac{C_6}{r^6} + \frac{C_8}{r^8} + \frac{C_{10}}{r^{10}} \right). \quad (15)$$

The coefficients can be calculated from the electron wavefunctions of a single atom. For the first three coefficients, calculations by Marinescu, Sadeghpour and Dalgarno give $C_6 = 1.472 \times 10^3 e_0 a_0^6$, $C_8 = 1.12 \times 10^5 e_0 a_0^8$, and $C_{10} = 1.11 \times 10^7 e_0 a_0^{10}$ [11]. The error bars are not discussed in Ref. [11], but subsequent papers (see e.g. Ref. [8]) have quoted an error of 5% in C_6 . At large r , the exchange energy falls off exponentially with r :

$$V_X(r) = -A_X e^{-r/a_X}, \quad (16)$$

In Ref. [12], the exchange parameters were determined empirically from data on the molecular energy levels near threshold in the spin-singlet and spin-triplet potentials. The values $A_X = 7.09 e_0$ and $a_X = 1.232 a_0$ give a good fit to the exchange energy down to distances as small as $r = 10 a_0$. The exchange term does not decrease to less than 10% of the dispersion term until r is greater than about $16.5 a_0$. Since there are few bound states whose wavefunctions extend beyond this distance, it will be crucial for our analysis to include the exchange term in the long-range potential.

IV. EFFECTIVE THEORIES FOR COLD ^{23}Na ATOMS

In this section, we construct effective potentials that reproduce the low-energy observables for two sodium atoms. We take the effective potential to have the following form:

$$V_{\text{effective}}(r) = V_{\text{long}}(r) + V_{\text{short}}(r) \quad (17)$$

$$= \begin{cases} V_C(r) + V_X(r), & r \geq r^*, \\ V_{\text{main}}(r) + V_{\text{tune}}(r; c_1, c_2), & r < r^*. \end{cases} \quad (18)$$

The long-range potential is the sum of the dispersion term $V_C(r)$ given in (15) and the exchange term $V_X(r)$ given in (16). We use the long-range potential for $r \geq r^*$, where $r^* = 10 a_0$. Below $r = r^*$, the potential changes discontinuously to the sum of the short-distance potential $V_{\text{main}}(r)$ and a tuning potential $V_{\text{tune}}(r)$. The tuning potential depends on parameters $\{c_1, c_2, \dots\}$ that can be tuned to reproduce low-energy data. The short-range potential is completely arbitrary. To demonstrate this, we will consider two potentials with completely different short-distance behavior. The first is a “realistic” potential, which is an accurate approximation to the true interatomic potential near its minimum. The second is a flat (“soft-core”) potential that has no repulsive core near $r = 0$. For each of these cases, we will construct an effective potential with 1 tuned parameter and ultimately then a more accurate effective potential with 2 tuned parameters (work in progress).

The two potentials are shown side by side in Figure 1. Note that they have very different behaviors. The depths of the wells differ significantly — $D_e/V_e \simeq 4.7$, where D_e is the depth of the Morse potential and V_e is the depth of the flat potential ($V_e = V_{\text{long}}(10a_e)$). Moreover, at small values of r they differ greatly as well — V_{Morse} is highly repulsive, effectively making the wavefunction 0 below about $4 a_0$, whereas V_{flat} allows a nonzero wavefunction in that region. One may ask why we do not consider the simplest possible main potential — 0. Certainly that is a valid choice. This, however, is a trivial choice as it does not allow any bound states to exist below $r = r^*$, a fact which is likely not a very wise choice.

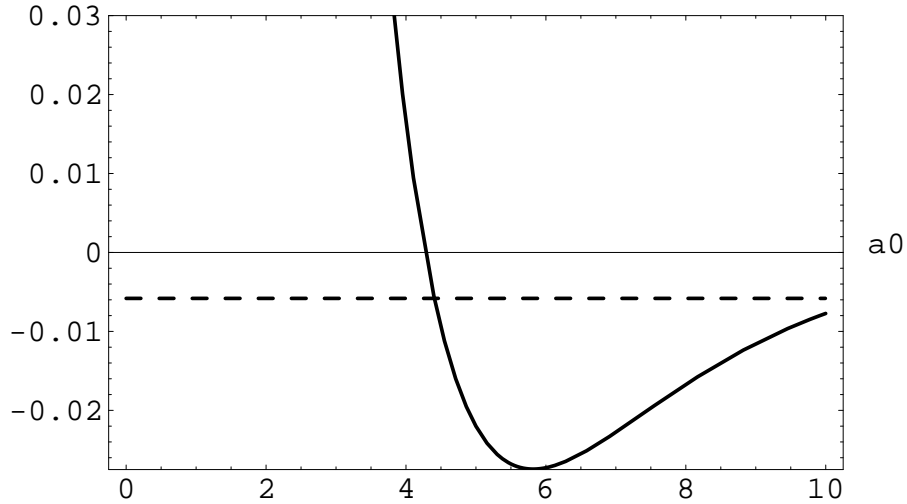


Figure 1. Comparison of two different main short-distance potentials. The two curves are $V_{\text{Morse}}(r)$ (solid line), $V_{\text{flat}}(r)$ (dashed line).

A. Realistic effective potential

For our realistic short-distance potential $V_{\text{main}}(r)$ we choose the Morse potential $V_{\text{Morse}}(r)$ given in (13). Its parameters have been adjusted to give the correct location r_e and depth D_e of the minimum of the potential and the correct energy splitting $E_{1,0} - E_{0,0}$ between the ground state and the first excited state. The effective potential with the tuning potential set to 0 is shown as a solid line in Figure 2. At $r = r^* = 10a_0$, the potential jumps discontinuously to the long-range potential $V_C + V_X$. With $c_1 = c_2 = 0$, the number of vibrational S-wave energy levels supported by the potential is 66. In spite of the fact that there are not 65 energy levels in the potential, we will label them starting from the top as $v = 64, v = 63, v = 62, \dots, v = 1, v = 0, v = -1$ in accordance with the standard notation for the corresponding energy levels in the true potential of starting the numbering from the top with 64.

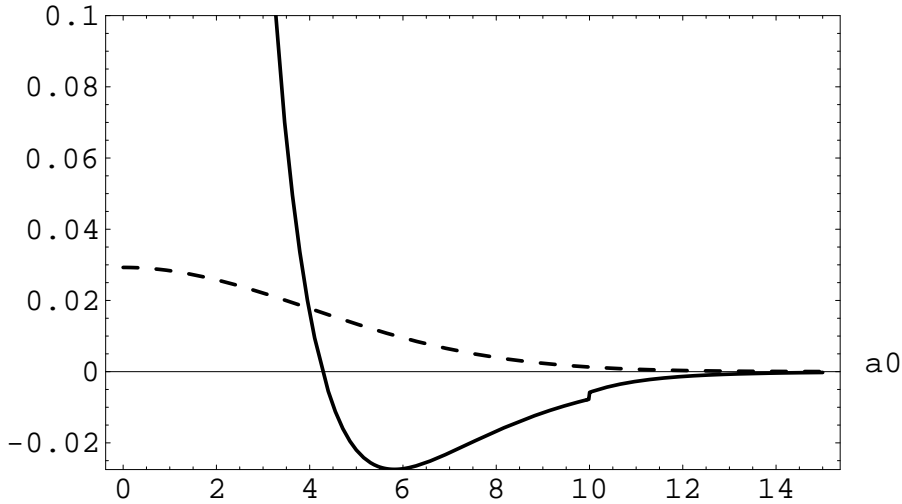


Figure 2. “Realistic” effective potential. The two curves are $V_{\text{effective}}(r)$ with $c_1 = c_2 = 0$ (solid line), $V_{\text{tune}}(r)$ with $c_1 = 1.84424$ and $c_2 = 0$ (dashed line).

From our analysis (see Ref. [4]) it is evident that the bound state energy differences are known much more accurately than the energies themselves, perhaps by as much as 10^2 . Therefore we tune the potential to the energy differences. Because we want to tune to the highest bound states possible and the top two ($v = 64$ and $v = 63$) have not been observed experimentally, we tune the short-distance parameters of the effective potential to reproduce the energy difference $E_{62,0} - E_{61,0}$ in the case of one parameter and expect to tune to $E_{62,0} - E_{61,0}$ and $E_{61,0} - E_{60,0}$ in the case of two parameters. The results of one-parameter tuning are shown in Figure 4. In it we plot the relative errors in energy differences against binding energy.

B. Flat effective potential

The short-distance part of the effective potential is completely arbitrary. To emphasize this fact, we will show that we can obtain an equally accurate⁷ description of low-energy observables using a potential that has the completely wrong behavior at short distances. We take the potential $V_{\text{main}}(r)$ to be constant all the way down to $r = 0$, so that it gives no short-range repulsion:

$$V_{\text{main}}(r) = V_C(r^*) + V_X(r^*). \quad (19)$$

We have chosen the short-distance potential so that it matches continuously onto the long-distance potential at $r = r^*$ when $c_1 = c_2 = 0$. If the tuning potential is nonzero, the total

⁷For an important qualification of this statement see p.14.

potential will have a small discontinuity at $r = r^*$. The effective potential with the tuning potential set to 0 is shown as a solid line in Figure 3. With $c_1 = c_2 = 0$, the number of vibrational S-wave energy levels supported by the potential is 66.

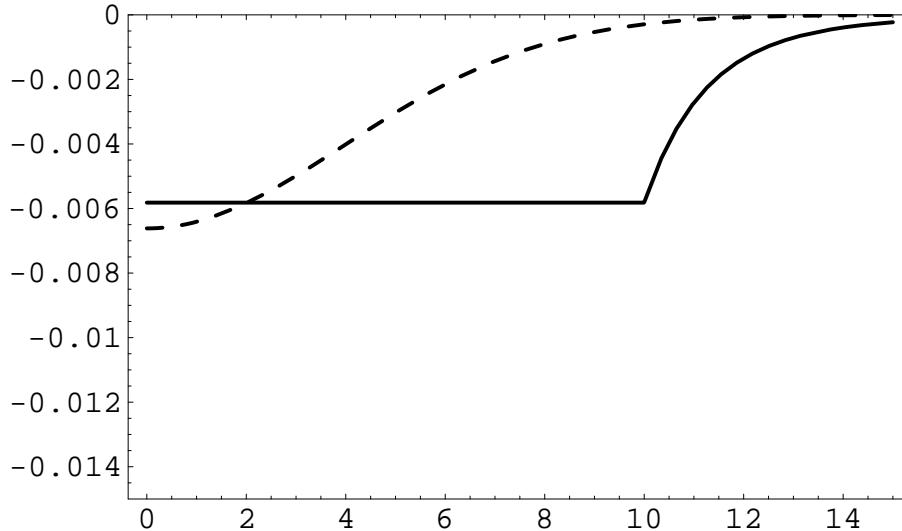


Figure 3. Flat effective potential. The two curves are $V_{\text{effective}}(r)$ with $c_1 = c_2 = 0$ (solid line), $V_{\text{tune}}(r)$ with $c_1 = -0.416792$ and $c_2 = 0$ (dashed line).

We similarly tune this potential to the energy difference between 62nd and 61st levels. Figure 5 presents the plot of our results for the flat potential.

V. LOW-ENERGY PREDICTIONS AND ERROR ANALYSIS

In the previous section, we tuned the short-distance parameters of the effective potentials to reproduce the energy difference $E_{62,0} - E_{61,0}$ in the case of one parameter. In this section, we examine the predictions of the effective theories for other low-energy observables.

A. Energy differences

The first low-energy observables that we consider are other energy differences $E_{v+1,0} - E_{v,0}$ that were measured in [14]. We expect that errors in the predicted energy differences will monotonically decrease with increasing energy, i.e., decrease with decreasing absolute value of energy. This means that the highest bound states are fitted best and have smallest errors. This makes perfect sense because lower-energy states are less sensitive to details of the short-distance potential than the higher ones. On a log-log plot the graph of relative errors against energy should be a straight line whose slope determines the scaling power of errors with energy.

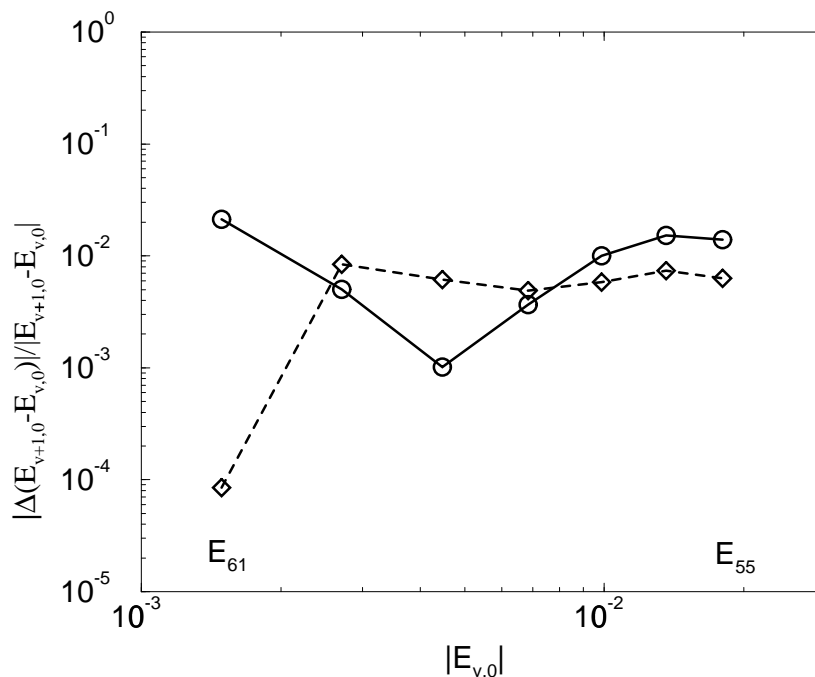


Figure 4. Fractional errors in the energy differences $|\Delta(E_{v+1,0} - E_{v,0})|/|E_{v+1,0} - E_{v,0}|$ as a function of the binding energies $|E_{v,0}|$ (in dimensionless units of $1/D_e$) for the realistic effective potential. The fractional errors are given for $c_1 = c_2 = 0$ (solid line), $c_1 = 1.84424$ and $c_2 = 0$ (dashed line).

Comparing the predicted energy differences with their measured values, we see that the errors behave in a more complicated and less systematic way than expected. The errors do not monotonically go down as energy goes up and there is not seen a significant improvement in accuracy, except in the highest energy difference of $|E_{62,0} - E_{61,0}|$.

Looking closely at both plots in Figure 3 we note that there is a big dip in errors around E_{59} , which is *inherent* in the untuned “realistic” potential. This provides a likely explanation for the little dip around roughly the same energy for the tuned potential. Around the energy of the 59th and 60th levels the errors try to decrease, but because of the nature of the underlying potential (as we saw in Figure 1 V_{main} dominates V_{tune}) they are forced up, hence the slight shift up. As expected, at the level to which we tuned the potential, the errors are clearly the smallest.

This behavior, of course, may also indicate the imperfectly known input into the theory. Perhaps the coefficients for the long-distance coulombic potential V_C and energy differences with which we are comparing our predictions need to be known much more accurately.

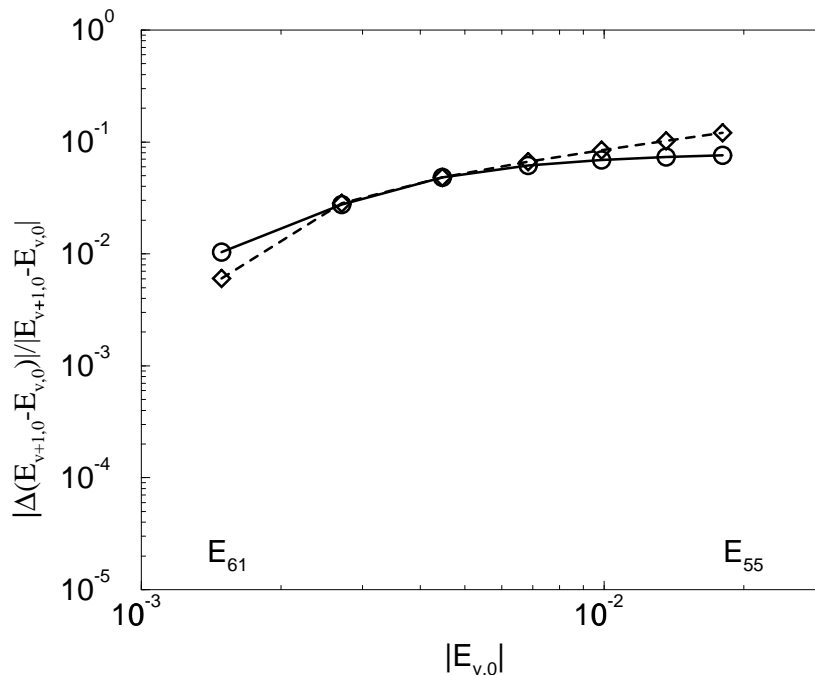


Figure 5. Fractional errors in the energy differences $|\Delta(E_{v+1,0} - E_{v,0})|/|E_{v+1,0} - E_{v,0}|$ as a function of the binding energies $|E_{v,0}|$ (in dimensionless units of $1/D_e$) for the flat effective potential. The fractional errors are given for $c_1 = c_2 = 0$ (solid line), $c_1 = -0.416792$ and $c_2 = 0$ (dashed line).

Here again we see that the tuning of the effective potential does not show a significant improvement over the untuned one. The general behavior of both curves, however, is more with the predictions of EFT. If we can treat the curves as roughly straight, then the slope is very small, perhaps $\simeq 0.27$. That goes against the claim of EFT that for one tuned parameter the errors should go as $|E_{v,0}|$.

To be sure, the one-parameter tuning of the flat potential is still in its early stages, so it is not surprising that this particular value for the coefficient c_1 does not work well. Perhaps there are others that will work much better. In addition, it is very likely that the inputs into the theory are not as accurate as expected and hoped, just like in the case of the “realistic” potential.

Note, however, a particular feature that accounts for the different behavior of the two potentials. Plotted on the same scale for better comparison, it is evident that the errors for the flat potential fare much worse than those for the “realistic” one. There should be no surprise in that; that is basically the essence of why one potential we called “realistic” and another not. The Morse potential is known to approximate quite accurately the true potential. Therefore it is only obvious that at any given level of tuning (with a fixed number of tuning parameters) its errors will be less than those of the flat potential. This was, therefore, the reason for our reservation about the equality of prediction accuracy for two different V_{main} potentials on page 10.

Nevertheless, we can still use an “unphysical” potential for our calculations. While at any level of tuning the more physical potential is expected to fare better, because of the systematic nature of growth of accuracy we only need to go to a finite number of tuning parameters to achieve desired accuracy for *any* potential. What this means, then, is that one might have to go to more parameters with V_{flat} than with V_{Morse} to achieve the same accuracy, but this number is always necessarily finite (for a finite accuracy).

B. Binding energies and Scattering lengths

Other low-energy observables we will eventually consider are the binding energies of the three molecular states nearest threshold and scattering lengths. Our analysis of the errors in the energy differences allows us to give an error bar on the predictions for the binding energies.

We will compare our predictions for the binding energies of the $v = 63$ and $v = 64$ levels with the theoretical predictions by Moerdijk and Verhaar [13]. They calculated the bound states closest to threshold in both the spin-singlet and spin-triplet potentials using a coupled-channel analysis that took into account the hyperfine interactions.

The final low-energy observable we will consider is the scattering length of the atoms. We will use our effective potentials to predict the scattering length in the absence of hyperfine interactions, which induce a coupling between the spin-singlet and spin-triplet channels.

VI. CONCLUSIONS

We have begun demonstrating the EHM approach that can be immensely useful for solving problems easier and better than ever before in low-energy physics. The work is still in progress, and it is too early to make any conclusions about whether the method really works; from the results presented here that is not evident. We are confident, however, that the approach does work and with good enough data on the long-distance potential and bound state energies we have no doubts that our predictions will conform to EFT expectations.

Further work remains to be done. That includes doing a more careful and thorough analysis of one-parameter tuning, the entire process of two-parameter tuning, testing our predictions against bound state energies themselves ($v = 62, \dots, 64$) and computing the scattering length a for ^{23}Na atoms. Estimating the error on that prediction we expect to predict a to significantly higher accuracy than ever before.

It is our great hope that atomic and molecular physicists will take the idea of EHM close to heart as we believe it will become a great tool in their arsenal.

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THINGS I DID THIS SUMMER FOR THE FIRST TIME IN MY LIFE!

CONCERTS:

- Country Concert — Kenny Chesney and Darryl Singletarry
- Oldies Concert — Credence Clearwater Revisited and the Beach Boys
- Rock Concert — Sugar Ray and Goo Goo Dolls

CLUBS:

- Country Club — “Club Dance”
- Techno Club — “Mecca”
- Dance Club — “Red Zone”

SHOWS:

- Mystery Dinner — “Cloak and Dagger”
- Wrestling — ECW

X-TREME SPORTS:

- Canoeing — Olentangy River
- Rock Climbing — “Vertical Horizons”
- Skydiving — “AerOhio”

PERSONAL:

- Earring — “Piercology”
- Dying Hair — light yellow :)