

# Ultracold Atoms

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PHYC30021 – Laboratory and Computational Physics 3



THE UNIVERSITY OF  
**MELBOURNE**

By R. A. Henry & J. P. Ellis  
School of Physics

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# I Introduction

In this experiment, you will use a simple version of the powerful numerical technique known as the **stochastic variational method (svm)** to find the ground state energy of two strongly-interacting cold atoms in a harmonic trap. The **svm** involves building up an approximation of the system's ground state by taking random samples of Gaussians (or other functions) with different length parameters, and using only the Gaussian which gives the most significant contributions to improve the approximation, while discarding the others. The two-body system is one of the simplest nontrivial examples of a few-body ultracold atomic system, and is one of the few nontrivial quantum systems which can be solved exactly, which will allow you to compare your numerical result to the known exact value.

## I.1 Ultracold Atom Physics

Ultracold atom physics is a relatively new field of study, but is now one of the most active and fruitful areas of modern physics research. An ultracold gas experiment involves somewhere between a handful and a few thousand atoms that are cooled to temperatures close to absolute zero, typically well below 1 K. Beyond this basic definition, there is a great variety of experimental and theoretical systems that fall within the ultracold atom field. Many novel and exotic quantum physical phenomena can be found in ultracold atom systems, such as **Bose–Einstein condensates (BECs)**, superfluidity, quantum magnetism, the quantum hall effect, many-body localisation and quantum phase transitions.

## I.2 Two-Body System

We will be considering a two-particle system which are both in a shared harmonic potential. The equation describing their interaction is

$$H = H_1 + H_2 + V(r_{12})$$

where  $H_i$  describes the interaction of the  $i$ th particle with the harmonic trap,

$$H_i := -\frac{1}{2m_i}\nabla_i^2 + \frac{1}{2}m\omega^2 r_i^2,$$

in which  $\mathbf{r}_i$  is the position of the  $i$ th particle; and  $V(r_{12})$  describes the interaction between the two particles where  $r_{12} := \|\mathbf{r}_1 - \mathbf{r}_2\|$  is the separation between the particles.

In this lab, we will be concerned with identical particles such that  $m = m_1 = m_2$  and we will also assume that they are in different spin states such that we need not worry about the (anti)symmetry of the Hamiltonian.

QUESTION 1: In the absence of  $V(r_{12})$ , what are the energy levels of this two-body system? Remember that we are describing a three-dimensional system.

QUESTION 2: Rewrite the two-body Hamiltonian in terms of the new coordinates:

$$\mathbf{r} := \sqrt{\frac{1}{2}}(\mathbf{r}_1 - \mathbf{r}_2), \quad \mathbf{R} := \sqrt{\frac{1}{2}}(\mathbf{r}_1 + \mathbf{r}_2).$$

You should find that the Hamiltonian can be separated into two:

$$H = H_{\text{com}} + H_{\text{rel}}$$

where  $H_{\text{com}}$  is (essentially) the centre-of-mass Hamiltonian and depends only on  $\mathbf{R}$ , and  $H_{\text{rel}}$  is the relative Hamiltonian and depends only on  $\mathbf{r}$ .

## 2 Scattering Theory

Before we can understand how the interaction term affects  $H_{\text{rel}}$ , we will need some of the basic concepts of scattering theory. In general, scattering theory is the study of how any sort of waves bounce off various objects or obstructions. The evolution of the wave is specified by some partial differential equation which includes a potential term that specifies the object, or *scatterer*. In quantum mechanics, these waves are wavefunctions which evolve under the Schrödinger equation and the scatterer is typically a larger (but still microscopic) structure such as an atomic potential.

Scattering theory is a large subject, and we will only cover some basic notions here. In this section, we will be considering an abstract quantum system in which a particle scatters elastically off some three-dimensional potential  $V(\mathbf{r})$ . In particular, we will be considering an interesting limit in which the potential can be described entirely by a single parameter, with all other details about the potential becoming irrelevant.

### 2.1 One-Dimensional Scattering

To get a little bit of intuition first, let's consider a one-dimensional system with a potential  $V(x)$ . Very far from the potential where  $V(x) \approx 0$ , the solution of the Schrödinger equation has the form of a plane wave:

$$\psi_{\text{L}} = Ae^{ikx} + Be^{-ikx} \qquad \psi_{\text{R}} = Ce^{ikx} + De^{-ikx}$$

where  $k = \sqrt{2mE/\hbar^2}$  and  $\psi_{\text{L,R}}$  describe the wave function to the left/right of the barrier.

If we consider the initial wave to be coming from the left, then  $A$  describes the original incoming wave,  $B$  is the reflected wave and  $C$  is the transmitted wave. As for  $D$ , in this instance it is zero but it is useful to leave it in for the sake of completeness. In this sense, the vector  $(B, C)$  describes the new wave generated by the scattering of the initial wave described by the vector  $(A, D)$ .

The 'scattering amplitude' describes the transition from the incoming wave to the outgoing wave. When there are finitely many incoming and outgoing states, the amplitude is described by a *scattering matrix*, or  $S$ -matrix which, in this one-dimensional case, is:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}.$$

In order that the  $S$ -matrix conserves probability, it must be unitary (that is  $S^\dagger S = 1$ ); and since the Schrödinger is invariant under time reversal, the  $S$ -matrix must be symmetric.

## 2.2 The Scattering Length and Universality

In section 2.1, we considered the scattering of a wave with wavenumber  $k$  scattering of a potential  $V(x)$  without really considering what  $V(x)$  is. It is possible that  $V(x)$  is an incredibly complicated function, but being a potential it will always be true that  $V(x) \rightarrow 0$  as  $x$  becomes sufficiently large. What happens then if the wavelength of the particle is much larger than the region where  $V(x)$  is non-zero? This will happen when  $k \rightarrow 0$  and thus when  $E \rightarrow 0$ , which is exactly what we have with ultracold atoms.

Your intuition for quantum mechanics and the way waves behave should tell you that the particle will not be able to see the intricacies of the potential. Without going into the derivation, it should not seem unreasonable that in the limit that  $k \rightarrow 0$ , the potential will resemble a solid sphere of radius  $a_s$ —and indeed the scattering theory does confirm this. This particular limit is called the *universality limit* specifically because all potentials are described solely by their scattering length and are independent of the exact details of the underlying potential. This the scattering of a van der Waals potential ( $\propto r^{-6}$ ) can be equally well described by a Gaussian potential or even a Dirac delta.

The scattering length can take any value from  $-\infty$  through to  $+\infty$ , with positive value indicating an attractive interaction; and negative values indicating a repulsive interaction. The larger the scattering length, the stronger the interaction between the particles with the limit at  $\pm\infty$  being the strongly interacting (or *unitary*) regime.

The potentials we will be interested in will have two parameters: an interaction length  $r_0$ , and a strength  $V_0$ . The actual scattering length is in general a function of these two parameters, though the derivation of the scattering length for various potentials is beyond the scope of this lab.

## 3 Analytic Solution

We now return to our two-body system and its Hamiltonian (section 1.2). As we are dealing with ultracold atoms, we are in the limit  $k \rightarrow 0$  and thus the potential describing how the two atoms interact can be solely described by the scattering length of the potential.

In order to arrive to an analytic solution, Busch, Englert, Rzażewski and Wilkens [1] take advantage of the universality limit and use a Dirac-delta potential as it has many nice analytical properties. To be precise, they use the regularized Dirac-delta potential

$$V(r_{12}) := 4\pi a_s \delta(\mathbf{r}_{12}) \frac{\partial}{\partial r_{12}} r_{12},$$

where the derivative needs to be introduced in order to ensure that the Hamiltonian is self-adjoint<sup>1</sup>.

Using this potential they are able to derive the following analytic expression which relates the scattering length to the energy levels of the system:

$$\sqrt{2} \frac{\Gamma(-E/2 + 3/4)}{\Gamma(-E/2 + 1/4)} = \frac{1}{a_s}.$$

Here,  $\Gamma(x)$  is the gamma function which is a generalization of the factorial function  $n! := n \cdot (n-1) \cdot \dots \cdot 2 \cdot 1$  to the entire complex plane (remember that  $\Gamma(n) \equiv (n-1)!$  for  $n \in \mathbb{N}$ ). Note that in order to make the solution easier, they have assumed some particularly ‘nice’ values of  $m$  and  $\omega$  in the potential (what are they?).

Any value of  $E$  which satisfies the above equation is an energy eigenvalue of the system for a given value of the scattering length  $a_s$ . The derivation of this equation is not reproduced here and can be found in the original paper.

**QUESTION 3:** Find the solutions of section 3. Note that it is not possible to analytically rewrite section 3 in the form  $E = \dots$ , so you will have to employ a root-finding algorithm.  
 What are the eigenvalues in the strongly interacting regime?  
 How do they eigenvalues changed based on  $a_s$  (both positive and negative)?

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<sup>1</sup>Had they not introduced the derivative, the 3D Hamiltonian would in fact only reproduce the non-interacting theory

## 4 Numerical Solution

We now know enough about the two-body problem to learn how an approximate numerical method can be applied to find an extremely accurate solution. This method we will use is the **SVM**. Variational methods are common and versatile tools for finding an approximate (and sometimes arbitrarily precise) solution to a **partial differential equations (PDEs)**. They work by making a initial guess about the general form of the solution called an *ansatz*, and then modifying the *ansatz* in such a way as to converge to the solution.

We will first be describing some of the numerical tools we need in order to implement the **SVM**, and then discuss at the end how the **SVM** algorithm works.

### 4.1 Using Basis Functions

Since we don't know the exact form of the solution, we must make some sort of guess, or *ansatz*, for the solution of the **PDE** (or we would not be resorting to numerical solutions). One overly simple *ansatz* would be try every function one after the other until we find the correct solution; however, the space of functions to cover is intractably large so unless we are able to narrow down the space of functions to test, this is simply infeasible.

Fortunately for us, we need not try every function but can instead use a *basis of functions* that can approximate a wide range of functions. If we can find the appropriate combination of basis functions and now how much of each function we need, we should be able to approximate our solution well. The solution will then be of the form:

$$|\phi\rangle = \sum_n |\phi_n\rangle,$$

where  $\{|\phi_n\rangle\}$  are the basis functions and  $c_n$  are the expansion coefficients.

We are free to choose from a very wide choice of basis functions, but for reason that should become apparent later, we will be using Gaussians of the form

$$\phi_n(\mathbf{r}) = \phi_n(r)Y_0^0(\theta, \phi) = \frac{1}{\sqrt{4\pi}}e^{-r^2/2w_n^2},$$

where  $w_n$  is the width of the Gaussian. Note that we are using the *s*-type solution ( $Y_0^0$ ), but it is possible to incorporate excited modes with  $\ell \neq 0$  by extending our basis to

$$\phi_{n,\ell,m}(\mathbf{r}) = \phi_n(r)Y_\ell^m(\theta, \phi).$$

By using many different widths, our basis will be able to capture variation in the true ground state on many different length scales, allowing a good approximation to be reached.



## 4.2 Determining Energy of Ansatz

So at this stage, we have our ansatz described by section 4.1 and we must compute the ground state energy associated with this ansatz and find the set of coefficient  $\{c_n\}$  which will be approximate the ground state.

Essentially, we need to find the values of the coefficients  $c_n$  which give the lowest energy i.e. we want to find the minimum of the energy  $E$  with respect to variations in  $c_n$ . To do this, we start with the definition of the energy  $E$ , and compute the infinitesimal change in energy  $\delta E$  corresponding to a small change in one of the coefficients,  $\delta c_i$ , then set  $\delta E = 0$ , corresponding to a local minimum in the energy:

$$\begin{aligned}
 E &= \langle H \rangle \\
 &= \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} \\
 &= \frac{\sum_{n,m} c_n c_m \langle \phi_n | H | \phi_m \rangle}{\sum_{n,m} c_n c_m \langle \phi_n | \phi_m \rangle} \\
 E \sum_{n,m} c_n c_m \langle \phi_n | \phi_m \rangle &= \sum_{n,m} c_n c_m \langle \phi_n | H | \phi_m \rangle \\
 E \sum_{n,m} c_n c_m S_{nm} &= \sum_{n,m} c_n c_m \mathcal{H}_{nm},
 \end{aligned}$$

where we have defined  $S_{nm} = \langle \phi_n | \phi_m \rangle$  and  $\mathcal{H}_{nm} = \langle \phi_n | H | \phi_m \rangle$ . These can be considered elements of some  $N$  by  $N$  matrices  $\mathcal{H}$  and  $\mathcal{S}$ , where  $N$  is the number of states in our basis. We now apply the perturbation to some  $c_i$ , which causes  $c_i \rightarrow c_i + \delta c_i$  and  $E \rightarrow E + \delta E$ . We compute the resulting differential in both sides of the equation, noting that we must apply the product rule on the left hand side:

$$\begin{aligned}
 \delta E \sum_{n,m} c_n c_m S_{nm} + \delta c_i E \sum_m c_m S_{im} + \delta c_i E \sum_n c_n S_{ni} \\
 = \delta c_i \sum_m c_m \mathcal{H}_{im} + \delta c_i \sum_n c_n \mathcal{H}_{ni} \\
 \delta E \langle \phi | \phi \rangle = 2\delta c_i \sum_n c_n (\mathcal{H}_{ni} - E S_{ni}),
 \end{aligned}$$

where we have recognised that the two summations are identical since  $\mathcal{H}$  and  $\mathcal{S}$  must be symmetric. Now, letting  $\delta E \rightarrow 0$ , viewing the summations as matrix multiplications, and writing the set of expansion coefficients as a set of vectors  $\mathbf{c}$ , we arrive at:

$$\mathcal{H}\mathbf{c} = E\mathcal{S}\mathbf{c}.$$

The last equation, section 4.2, resembles a matrix eigenvalue equation for the matrix  $\mathcal{H}$ , where  $E$  is a diagonal matrix of eigenvalues, except that we have an additional matrix  $\mathcal{S}$ . This is known as a *generalized eigenvalue equation*, with the matrices  $\mathbf{c}$  and scalar  $E$

being the generalised eigenvectors and eigenvalues respectively. We could multiply both sides by  $\mathcal{S}^{-1}$  and quickly reach a regular eigenvalue equation. However, it is actually more computationally efficient to solve the generalised eigenvalue equation than to compute the inverse of a large matrix, so we leave it as is.

Finally, given an initial set of basis functions  $\{\phi_n\}$ , we have found the optimal coefficients  $\{c_n\}$  such that the linear combination  $\sum_n c_n \phi_n$  approximates the ground state best. We were able to do so because the matrices  $\mathcal{H}$  and  $\mathcal{S}$  only depend on the basis states and the Hamiltonian, and the calculation of  $\{c_n\}$  came down to just a linear algebra problem.

QUESTION 4: What information does the matrix  $\mathcal{S}$  encode?

#### 4.2.1 Calculating Matrix Elements

As mentioned above, we must calculate the matrices  $\mathcal{H}$  and  $\mathcal{S}$  which are defined by

$$\mathcal{S}_{nm} = \langle \phi_n | \phi_m \rangle, \quad \mathcal{H}_{nm} = \langle \phi_n | H | \phi_m \rangle.$$

Since we know the form of the basis functions in position space (section 4.1), the evaluation of these brackets becomes an integral over space. Explicitly:

$$\begin{aligned} \mathcal{S}_{nm} &= \langle \phi_n | \phi_m \rangle \\ &= \int_{4\pi} d\Omega \int_0^\infty r^2 dr \phi_n(\mathbf{r}) \phi_m(\mathbf{r}) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_{nm} &= \langle \phi_n | H | \phi_m \rangle \\ &= \int_{4\pi} d\Omega \int_0^\infty r^2 dr \phi_n(\mathbf{r}) H_{\text{rel}} \phi_m(\mathbf{r}) \end{aligned}$$

The difficulty of these integrals depends entirely on our choice of basis functions. One could resort to using numerical integration; however, as we have  $3d$  integrals, the computation time will increase very rapidly. To be more precise, if we use a simple trapezoidal rule numerical integration with  $N$  subdivisions, these integrals will require summing up  $N^3$  points, and this has to be repeated for *every pair of basis functions*!

Fortunately, the choice of basis functions is ours and a judicious choice of basis functions might make these integrals analytically solvable. One set of very nice functions to work with are Gaussians since the product of two Gaussians is a Gaussian, the derivative of a

Gaussian is a Gaussian (multiplied by a polynomial), and the integral of a Gaussian has a simple analytic form:

$$\mathcal{I}(a, n) := \int_0^\infty x^n \exp(-ax^2) dx = \frac{1}{2\sqrt{a^{n+1}}} \Gamma\left(\frac{n+1}{2}\right).$$

If we also use a Gaussian for the potential  $V(r_{12})$ , then everything is a Gaussian and everything can be integrated analytically.

**QUESTION 5:** Express the matrix elements  $\mathcal{S}_{ij}$  and  $\mathcal{H}_{ij}$  in terms of the Gaussian integral  $\mathcal{I}(a, n)$ . Remember to use spherical coordinates!

### 4.3 Generation of Basis States

At this stage, we are able to calculate the optimal set of coefficients  $\{c_n\}$  given a set of basis functions  $\{\phi_n\}$ ; however, how are we to find the set of basis functions  $\{\phi_n\}$ ?

This is where the *stochastic* aspects comes into play in this lab because we simply don't know. Lacking any other insight, then we might as well use trial-and-error and simply pick basis functions at random (hence *stochastic*).

This creates a significant problem though because programs like to be *deterministic*. As coders, we like to know exactly what the code will do when, what kind of inputs we will get, etc. which unfortunately won't happen in a stochastic algorithm. As a result, we have to take a lot more care to consider *all edge cases*.

The general idea of the algorithm is as follows:

1. Begin with a set of  $N$  states  $\{\phi_n\}$
2. Extend the basis by adding one new state, picked at random.
3. Calculate the new ground state energy. If the new ground state is lower than the previous one, keep the new state in the basis.
4. Go back to step 1.

Note an easy optimization to the above algorithm would be to try a large number of random states and pick the best out of all of them (instead of stopping at the first improvement).

As mentioned above though, great care must be taken to take into account different edge cases. For example, what will happen if:

- the basis is extended by adding a new state that is already in the basis?
- the new basis that is added is invalid?
- the ground state energy becomes negative?
- there is a numerical instability in the generalized matrix equation?

There is one last aspect to discuss before moving on: how should the random state be picked? As we have a spherically symmetric system, all our Gaussian are centered at the origin so the basis functions only vary in their width; as a result, selecting a random basis to add boils down to selecting a random width. The width itself can take any value in  $[0, \infty)$ , but do you expect that all choices from this interval be applicable for our system? An incorrect choice of interval means that it may take a very large number of trials before finding a new set of basis functions that improves the ground state energy, or worse yet, might mean that you never can approximate the ground state solution.

### 4.3.1 Convergence Conditions

We now have the ingredients of an algorithm that builds up a successively better approximation for the ground state energy, but how will we know when to stop? The simplest approach is just to limit the total number of states that will be used, a proscription which will suffice for this project. Note that in some cases, adding additional basis states when the system is close to convergence will cause the simulation to break down and give rapidly decreasing negative eigenvalues.

There are of course more advanced convergence conditions that will yield more consistent results. A simple but effective approach is to calculate the relative (i.e. percentage) difference in the energy compared to the previous step, and only accept new states that give a relative difference above some threshold and if no such state can be found the simulation ends.

## 4.4 Extrapolating to Zero-Range

Our algorithm relies on using a Gaussian potential in the Hamiltonian, of the form

$$V_0 \exp\left(-\frac{r^2}{2r_0^2}\right),$$

where  $r_0$  is the interaction length, and  $V_0$  determines the strength of the interaction. Physically, the most appropriate value of  $r_0$  will be extremely small, so small in fact that  $r_0^{-2}$  will become impractically large for a computer to handle. For this reason, we will be computing the ground state energy for a set of larger  $r_0$  and extrapolate to  $r_0 = 0$ . Fortunately for us, the dependence on the ground state energy on  $r_0$  is linear (for the values of  $r_0$  we are concerned with), so a straight line fit will suffice.

The limit  $r_0 \rightarrow 0$  will coincide with  $a_s \rightarrow \infty$  which will allow you to compare your numerical result with the analytical result found earlier.

## 4.5 Writing Your Simulation

You will be writing your code in Python. Some skeleton code is provided, though you are free to write your own code.

One thing you must keep in mind is that we are using a lot of random states. This means that functions aren't always guaranteed to work. This means that when you functions must have a way of returning failures (for example, by return `None` instead of a number), and then when calling on functions which might fail, you must handle failures too.

For example, when building up your basis, you might be tempted to simply have:

```
1 while number_of_states < desired_number_of_state:
2     # Find a new state that improves fit and add it to the system
```

but what happens if you are no longer able to find new states that improve the fit to the ground state before the desired number of states is reached?

Also be aware that when adding more states, your matrices can become numerically unstable and finding eigenvalues will result in an error. Since we know this error might occur, we must handle it appropriately in Python. This is described within the skeleton code provided.

QUESTION 6: At each step of the simulation, you re-solve the generalised eigenvalue problem to obtain  $N$  eigenvalue, where  $N$  is the number of basis functions at that step. The first eigenvalue is the ground state energy. What do the other eigenvalues represent? Are their values useful?

QUESTION 7: Plot the ground state energy as a function of the size of your basis and comment on its convergence. What about plotting the first or even second excited state as a function of the basis size.

Note that given this is stochastic, it might be worth repeating this many times and then aggregating the data before plotting it.

QUESTION 8: What is the probability density of the ground state you have found?

## 4.6 Extensions

The lab can be extended in one of two fairly obvious ways. Firstly, one can easily look at the effect of changing  $\omega$  and  $m$  on the energy levels.

Another extension would be to consider a slightly different basis. In this lab, we considered only  $\ell = 0$  solutions; but what if we used  $\ell = 1$  (i.e.  $p$ -wave)? What if we combined with  $\ell = 0$  and  $\ell = 1$ ?

#### 4 Numerical Solution

Alternatively, you could also extend the basis from purely Gaussians to Gaussians multiplied by a polynomial:

$$\phi_{n,a,b} = \frac{(1 + ar + br^2)}{\sqrt{4\pi}} e^{-r^2/2w_n^2}$$

This is slightly more complicated to handle than pure Gaussians, but still has the nice properties discussed in section 4.2.I.

# References

- [1] T. Busch, B.-G. Englert, K. Rzażewski and M. Wilkens, ‘Two cold atoms in a harmonic trap’, *Foundations of Physics* **28**, 549–559 (1998).