

Variational principle characterization of simple atomic and molecular systems.

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I. INTRODUCTION

In practice, the end goal of an investigation into the quantum mechanics of a physical system is often to find the ground state energy E_0 . Like any observable, we can calculate this quantity as an expectation value

$$E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle = \int \psi_0^*(\mathbf{r}) \hat{H} \psi_0(\mathbf{r}) d\mathbf{r}.$$

However, it is not always possible to determine the ground state wavefunction $|\psi_0\rangle$ analytically or easy to approximate it numerically. In these cases, there is an extremely powerful tool known as the variational principle which allows us to estimate the ground state energy within the same expectation value formalism. It can be easily proved [1] that the ground state of any Hamiltonian \hat{H} satisfies

$$E_0 \leq \langle \psi | \hat{H} | \psi \rangle$$

for any normalized wavefunction $|\psi\rangle$. In practice we use a "trial wavefunction" that depends on various tunable parameters

$$|\psi_T\rangle = \psi(\mathbf{r}, a, b, \dots)$$

so that we can then minimize $\langle H \rangle = \langle \psi_T | \hat{H} | \psi_T \rangle$ with respect to these parameters. Then, the variational principle guarantees that the smaller the minimum of $\langle H \rangle$ the closer we are to the true ground state energy.

II. APPROACH

The variational principle as explained so far may seem like a computationally simple method consisting of integration and optimization. However, considering that it is often employed to find ground states of n particle wavefunctions according to

$$E_0 \leq \int \psi_T^*(\mathbf{r}_1 \dots \mathbf{r}_n) \hat{H} \psi_T(\mathbf{r}_1 \dots \mathbf{r}_n) d\mathbf{r}_1 \dots d\mathbf{r}_n$$

the computational power required to evaluate these $3N$ dimensional integrals with conventional methods such as Gaussian quadrature can be immense. Thus we turn to two closely related computational methods to facilitate the evaluation of these integrals within the variational principle scheme.

A. Monte Carlo Integration

Like any numerical integration scheme, the Monte Carlo method involves replacing the integral with a sum. However, an important distinction is that rather than summing over a simple linear mesh of domain points like we would in a rectangle integration scheme, we instead sample points from a probability density function (PDF). Any PDF is acceptable to use in a Monte Carlo method, but of special utility are PDFs which are chosen to fit the function to be integrated. The use of a PDF such as a gaussian to integrate a function which reaches its maximum at $x = 0$ and goes to zero at its endpoints, i.e. using a PDF with similar features to the integrand, is called importance sampling [2]. The general formula for rewriting an integral over $F(y)$ as a sum using importance sampling is [2]:

$$I = \int_a^b F(y) dy = \int_a^b \frac{F(y) \text{PDF}(y)}{\text{PDF}(y)} dy =$$

$$\int_{a'}^{b'} \frac{F(y(x))}{\text{PDF}(y(x))} dy = \frac{1}{N} \sum_{i=1}^N \frac{F(y(x_i))}{\text{PDF}(y(x_i))}$$

where the PDF is normalized and similar to the integrand and each x simply comes from a uniform random number distribution and is used to generate y values.

This procedure works whether y is a scalar or a 20-dimensional vector. In fact, it can be shown that using a Monte Carlo method, the standard deviation on an N term estimation of the integral is

$$\sigma_N = \frac{1}{\sqrt{N}}.$$

This result is independent of the dimensionality of the integral but depends only on the sample size N . [2]. This is not true of other integration methods, whose uncertainties increase in higher dimensions, and so must employ absurdly high N to achieve convergence of these integrals, but with Monte Carlo, the necessary N values and thus the required computational power will be much lower.

B. Metropolis Algorithm

The use of Monte Carlo methods allows us to bypass many of the difficulties of high dimensional integrals, but

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#### in the metropolis function
#### x is the array of sample states that we want to
construct
#### the initial state x[0] is already determined

# go thru the N steps of the walk
for i in range(1,N):

    # get vector of the new step
    delta=np.random.normal(0,1,n);
    xint=x[i-1,:]+delta; # add to the old state to get
        the trial new state

    # get value of pdf at current state and trial state
    pdf_of_trial= PDF( xint, *pdf_args );
    pdf_of_current= PDF( x[i-1], *pdf_args );
    R=pdf_of_trial/pdf_of_current; # ratio determines
        how likely we are to make this step

    # always make steps from less to more probable states
    if (R>=1):
        x[i,:]=xint

```

FIG. 1. Code snippet showing how we use the ratio R of the trial to current PDF to ensure that steps to a higher PDF value are always accepted.

we now face the problem of how to generate samples for the sum. The best way of doing this is to have the sample set reflect the physics of the specific problem. As such, the norm squared of the wavefunction $|\psi|^2$ which is also the PDF of the particle will play an important role. A simple way of sampling the PDF is to perform a random walk. Letting a walker make random movements "backward" and "forward" along each axis of the parameter space could provide a good sampling, but could also lead to a bad one, owing to its randomness.

The metropolis algorithm places constraints on the random walk so that it accurately samples the system. This algorithm is a Markov process in that each step does not depend on anything but the current state [2]. These processes have the helpful property that they go toward an equilibrium distribution after enough time [2]. The first constraint, as shown in Figure 2, is to always accept steps towards regions of the parameter space where the PDF is greater, ensuring that we sample these regions, which are of the greatest importance to the integral.

The secondary constraint is to sometimes accept moves toward regions of lower probability. This means that we do not forget these regions entirely, but also keeps us from getting stuck in them and overrepresenting their importance. This process is detailed in the code in Figure 2.

III. BENCHMARKING

A. Hydrogen Atom

The metropolis algorithm code detailed above is useful for performing variational principle calculations in many

```

#### still in the metropolis function
#### still looping over i|

# sometimes make steps from more to less probable
states
else:
    alpha=np.random.uniform(0,1,1); # random
        threshold for taking less probable step
    if (R>alpha): # step is accepted
        x[i,:]=xint; # new state is trial state
    else: # step is rejected
        x[i,:]=x[i-1,:]; # new state is current state
        rejections += 1;

```

FIG. 2. Code snippet showing how we handle steps to less probable states.

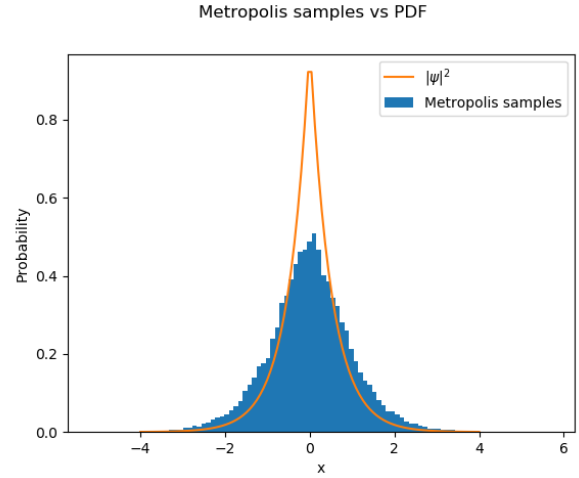


FIG. 3. At $N = 10^5$ samples, the metropolis algorithm shows good agreement with the PDF of the wavefunction itself. The samples generated are vectors in $\hat{x}, \hat{y}, \hat{z}$, but only the \hat{x} axis is plotted. The sample set will never fully match the PDF at $x = 0$ as a tradeoff for ensuring the exterior regions are properly represented.

particle systems, but before we proceed we should investigate the convergence of the method with respect to sample size N . The hydrogen atom is a very simple, single particle case that can serve this purpose.

Using the known ground state wavefunction of the hydrogen atom,

$$\psi_0 = Ae^{-r_j/a_0} \quad (1)$$

where a_0 is the Bohr radius, we should be able to employ the metropolis code to calculate observables of the system [1]. Before doing this, we must verify that the metropolis sampler is generating states that appropriately reflect the PDF. This is confirmed in Figure 3.

Since we are using the exact wavefunction, we are guaranteed to always calculate the correct $\langle H \rangle$, but since this wavefunction is not an eigenstate of the position operator, we can investigate the convergence of the observable

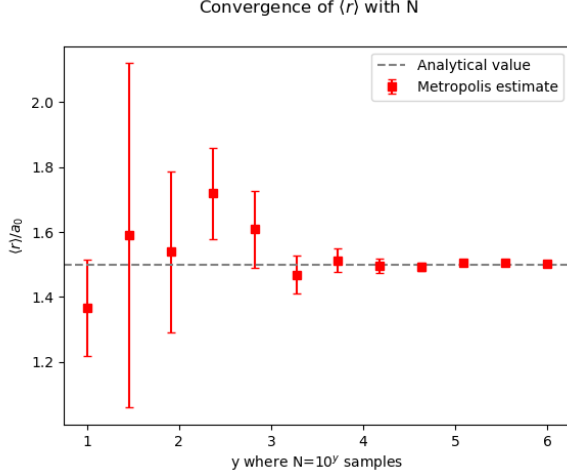


FIG. 4. Metropolis calculation vs sample size N . The analytical result for $\langle r \rangle$ in the hydrogen atom is $1.5a_0$ [1]. The 3σ error is shown where $\sigma = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} / \sqrt{N}$

$\langle r \rangle$. This is helpful in determining reasonable values of N to use going forward. The metropolis estimation of $\langle r \rangle$ vs N shown in Figure 4 shows that 10^5 to 10^6 samples is a good range for achieving convergence to the correct value and for minimizing the uncertainty..

B. Helium Atom

Having benchmarked the metropolis sampler, we next ensure that the code for determining the minimum of $\langle H \rangle$ by the variational principle is satisfactory. The case of a helium atom (2 protons, 2 electrons) is well suited for a test case of our method because it concerns multiple particle integrals but is also well studied. In particular, the fact that we can write the hamiltonian as [1]:

$$\begin{aligned} \hat{H} &= \frac{-\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0} \left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right) \\ &= \hat{H}_H(\mathbf{r}_1) + \hat{H}_H(\mathbf{r}_2) + \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|}, \end{aligned} \quad (2)$$

where \hat{H}_H is a hydrogen-like Hamiltonian, is significant. It suggests that the hydrogen ground state (Equation 1) would be a reasonable choice for the individual particle wavefunction. We can then construct the trial wavefunction to be the product of the individual particles

$$\psi_T = A e^{-r_1/a} e^{-r_2/a} \quad (3)$$

where the Bohr radius has been replaced by the tunable parameter a .

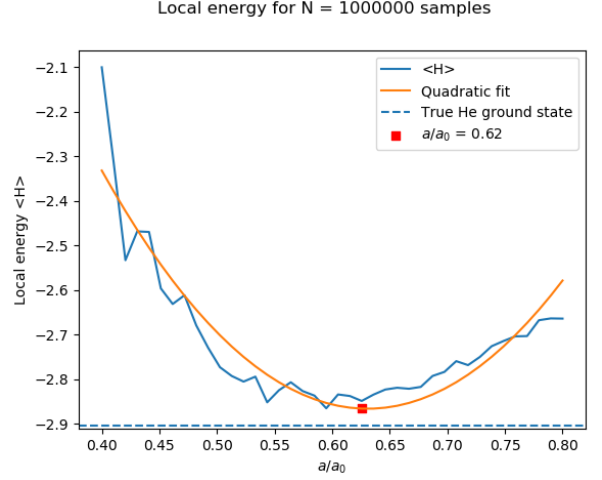


FIG. 5. Local energy sweep over tunable parameter a with accompanying second order fit to determine the minimum of the data. The resulting value of $\langle H \rangle < -2.85$ is in fairly close agreement with the experimentally determined ground state of -2.90 .

We simplify units by setting $m = e = \hbar = 4\pi\epsilon_0$ in light of which the Bohr radius is simply one [2],

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 1.$$

Then we likewise move to the dimensionless energy variable

$$\lambda = \frac{ma_0^2 E}{\hbar^2},$$

noting that $\lambda = -\frac{1}{2}$ is the ground state energy of hydrogen in this unit system [2]. Then by comparison of the experimentally determined ground state of helium in eV we can determine $\lambda = -2.90$ is the helium atom ground state in this unit system. As a benchmark of our metropolis method local energy calculation, we will see how close we can get to this value by tuning the parameter a in Equation 3 and looking for the minimum.

We begin with a coarse sweep of the region $0.1 < a/a_0 < 1$, motivated by the thinking that with an effective nuclear charge higher than that of hydrogen, helium should have a smaller atomic radius, and thus $a < a_0$. This allowed us to pinpoint the region $0.4 < a < 0.8$, so we proceeded with a fine sweep of this region with $N = 10^6$ samples to reduce statistical noise. Fitting the result to a quadratic allowed us to determine a/a_0 as the value minimizing the local energy, as shown in Figure 5.

IV. HYDROGEN MOLECULE

Aside from the interactions we saw in the case of the helium atom, in a diatomic hydrogen molecule (another system of two protons and two electrons) we must also

consider the electromagnetic repulsion between the two protons and cross attractions between electrons and both protons. In this case, using \hat{H}_H as before, \mathbf{r}_1 and \mathbf{r}_2 to refer to the positions of the two electrons, and \mathbf{R}_1 and \mathbf{R}_2 to refer to the positions of the two protons, the hamiltonian for the system is [1]:

$$\hat{H} = \hat{H}_H(\mathbf{r}_1, \mathbf{R}_1) + \hat{H}_H(\mathbf{r}_2, \mathbf{R}_2) + \frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{1}{|\mathbf{R}_1 - \mathbf{R}_2|} - \frac{1}{|\mathbf{r}_1 - \mathbf{R}_2|} - \frac{1}{|\mathbf{r}_2 - \mathbf{R}_1|} \right). \quad (4)$$

To simplify, let's position the first nucleus at the origin and the second at $\mathbf{R}_2 = R\hat{\mathbf{x}}$ so that $\mathbf{R}_1 - \mathbf{R}_2 = R$.

A. Hydrogen Atom Trial Wavefunction

In picking a trial wavefunction we again take our cue from the fact that the Equation 4 can also be partly separated into hydrogen hamiltonians, so we should again incorporate the hydrogen ground state wavefunction. These separated hamiltonians $\hat{H}_H(\mathbf{r}_1, \mathbf{R}_1)$, $\hat{H}_H(\mathbf{r}_2, \mathbf{R}_2)$ have ground state eigenfunctions

$$\psi_0(\mathbf{r}_1) = e^{-r_1/a} \text{ and}$$

$$\psi_0(\mathbf{r}_2 - R\hat{\mathbf{x}}) = e^{-|\mathbf{r}_2 - R\hat{\mathbf{x}}|/a}$$

respectively in our chosen coordinate system. Each individual particle wavefunction is the eigenfunction of a different separated hamiltonian, so we multiply them together to find the total trial wavefunction. However, we must also consider that the two electrons, being fermions, must have a wavefunction that is antisymmetric under interchange. We proceed by assuming that the electron spins are in the antisymmetric singlet state, so that the spatial wavefunction must be symmetric. The trial wavefunction is then

$$\psi_T = A(\psi_0(\mathbf{r}_1)\psi_0(\mathbf{r}_2 - R\hat{\mathbf{x}}) + \psi_0(\mathbf{r}_1 - R\hat{\mathbf{x}})\psi_0(\mathbf{r}_2)). \quad (5)$$

Here A is a normalization constant, but need not be determined as it will be divided back out in the Monte Carlo integration. From this it is straightforward to have the metropolis algorithm generate samples from the PDF $|\psi_T|^2$ in the 6D vector space $[\mathbf{r}_1, \mathbf{r}_2]$.

1. Minimization of $\langle H \rangle$

Although this trial wavefunction is distinct from the case of the He atom, we still proceed by finding the minimum of the local energy with respect to the tunable

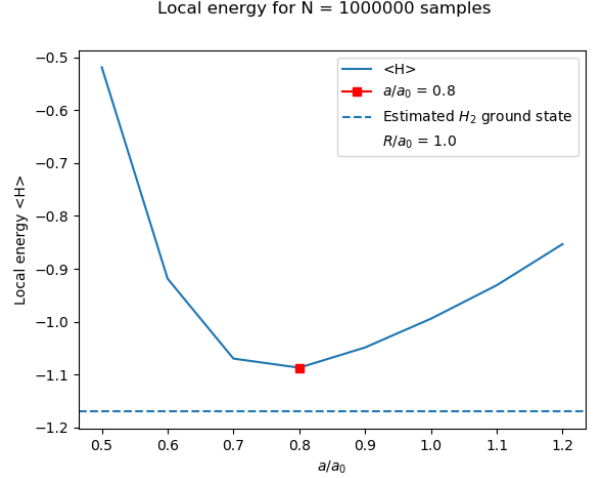


FIG. 6. Hydrogen molecule local energy sweep over tunable parameter a for interatomic distance fixed at $R = a_0$. We used a Metropolis sample of size $N = 10^6$. The resulting local energy minima at $a = 0.8a_0$ is well above the true ground state, indicating that this is not an optimal value of R .

parameter a . An example of such a calculation is shown in Figure 6. Note that we have assumed that a will have the same value for each atom in the molecule, which is justified by the fact that the two electrons and protons are identical particles.

For the H_2 molecule we are interested in determining not only in the minimum energy but also the equilibrium bond length R_{bond} , corresponding to the value of R that results in a stable covalent bond. The interatomic distance R is an input of the Hamiltonian, not a tunable parameter of the trial wavefunction, but we may bend the rules here by treating it as the latter and finding the its value that minimizes $\langle H \rangle$. This is justified because the physical system will find the bond length that allows it to reach the lowest energy state. By repeating the sweep over a for every R in a mesh of R values we are able to estimate the interatomic distance that minimizes the local energy. This will correspond to the equilibrium bond length of the molecule. The minimization procedure shown in Figure 7 gives a good estimate of this quantity. We then proceeded with a quadratic fit of the region around the minimum, $1.1 < R/a_0 < 1.7$, to determine the equilibrium bond length to be $R_{bond} = 1.44a_0$. In SI units, this result of $R_{bond} = 0.762\text{\AA}$ agrees well with the experimentally reported interatomic distance 0.742\AA [3].

2. Energy levels of the molecule

The bond length R_{bond} determined above is a useful physical quantity in its own right when one considers the accessible kinetic energy modes of the molecule. For any diatomic molecule such as H_2 , the rotational energy levels

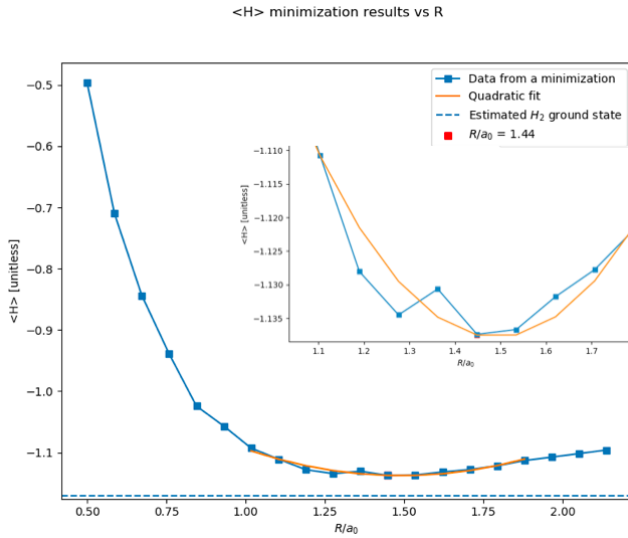


FIG. 7. Hydrogen molecule local energy sweep over interatomic distance R . The region near lowest $\langle H \rangle$ was fit with a quadratic, shown in the inset. Note that the Metropolis sample size was decreased to $N = 5 \times 10^5$ to decrease computation time.

are quantized according to

$$E_{rot} = \frac{J(J+1)\hbar^2}{2I}, \quad (6)$$

$$\text{where } I = \mu R^2 = \frac{m_p m_p}{m_p + m_p} R^2 = \frac{1}{2} m_p R^2$$

is the moment of inertia of the molecule, $m_p = 1830m_e$ is the mass of the proton, and J is the rotational angular momentum quantum number [4]. With the results of the previous section, we can calculate the rotational energy level spectrum to be

$$E_{rot} = \frac{J(J+1)(1.05 \times 10^{-34})^2}{1830 \times 9.11 \times 10^{-31} (1.44 \times 5.29 \times 10^{-11})^2}$$

$$= J(J+1) \times 1.14 \times 10^{-21} \text{ J}, \quad J = 1, 2, 3 \dots$$

where we have switched to SI units. As a result, the rotational energy of the molecule will be activated at a temperature given by

$$k_B T = 2 \times 1.14 \times 10^{-21} \text{ J} \rightarrow T = 165.2 \text{ K}.$$

We can also ask the same question for the vibrational energy levels. The x^2 fit of the data in Figure 7 can be used to extract the spring constant $k = 0.360$. Then it is well known that for angular frequency

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{0.36}{0.5 \times 1830}} = 0.0198$$

the vibrational energy levels are given by

$$E_{vib} = \hbar\omega(n + \frac{1}{2}) = 0.0198(n + \frac{1}{2}).$$

Since the conversion to SI energy is accomplished by

$$0.0198 * \frac{-13.6 \text{ eV}}{-0.5} * \frac{1.60 \times 10^{-19} \text{ J}}{1 \text{ eV}}$$

then the SI unit energy levels are

$$E_{vib} = 8.63 \times 10^{-20} (n + \frac{1}{2}) \text{ J}.$$

As a result we can finally find the temperature at which these modes are activated, namely

$$k_B T = \frac{1}{2} * 8.63 \times 10^{-20} \rightarrow T = 3130 \text{ K}.$$

We may also determine the frequency of the ground state vibrational mode according to

$$E_{vib} = \frac{1}{2} * 8.63 \times 10^{-20} = h\nu = hc\tilde{\nu}$$

and arrive at $\tilde{\nu} = 2170 \text{ cm}^{-1}$. Again this is in satisfactory agreement with the experimental value of $\tilde{\nu} = 2080.6 \text{ cm}^{-1}$ [3].

B. Harmonic Oscillator Trial Wavefunction

A second choice of trial wavefunction is motivated by the fact that each electron will be close to the nuclei. We thus expect the probability distribution of the j^{th} electron to approach 0 as $|\mathbf{r}_j| \rightarrow \infty$, a condition ψ_0 satisfies, but it does so rather slowly. A faster dropoff is achieved by using the individual particle trial wavefunction

$$\phi_0 = Ae^{-(r_j/a)^2}. \quad (7)$$

Note that for dimensional correctness, the tunable parameter a , which has units of length, must also be squared. We often refer to this as the harmonic oscillator trial wavefunction because of the $\exp(-r^2)$ dependence which resembles the solutions of that system. To achieve an antisymmetric total wavefunction in combination with the antisymmetric spin singlet, we follow the same procedure as Equation 5 to construct a symmetric spatial wavefunction:

$$\phi_T = A(\phi_0(\mathbf{r}_1)\phi_0(\mathbf{r}_2 - R\hat{\mathbf{x}}) + \phi_0(\mathbf{r}_1 - R\hat{\mathbf{x}})\phi_0(\mathbf{r}_2)). \quad (8)$$

As before, we do not need to find the value of the normalization constant A in order to determine $\langle H \rangle$.

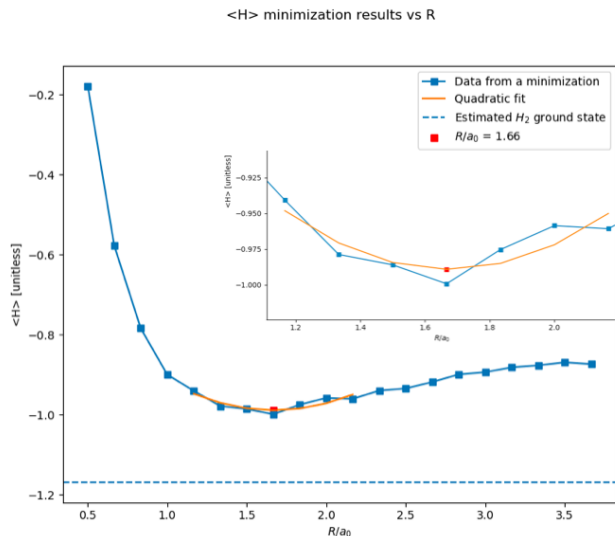


FIG. 8. Local energy vs interatomic distance with the harmonic trial wavefunction ϕ_T . Again, a reduced sample size of $N = 5 \times 10^5$ was used. The resulting local energy minimum is somewhat higher than in Figure 7.

1. Minimization of $\langle H \rangle$

The procedure for this trial wavefunction is the same as above. We first look at a scan over a for a fixed value of R . Then in Figure 8 we repeat this for a mesh of R values to arrive at $R_{bond} = 1.66a_0$. This result of 0.878\AA is on the same order of magnitude as the experimental result but is much farther away than our previous calculation [3]. This indicates that the trial wavefunction ϕ_T is not as close to the true ground state solution to Equation 4 as ψ_T , which is also apparent from the fact that the latter minimizes $\langle H \rangle$ at -1.14 , much lower than the former, which only achieves $\langle H \rangle = -1.00$.

2. Energy levels of the molecule

The physics of the energy levels of the molecule is presented in the calculations made in Section IV A 2, which we will only need to modify based on the differing results for this trial wavefunction. The new interatomic distance means the correction $(1.83/1.44)^2$ must be applied to the moment of inertia calculation. As a result, the rotational energy levels become

$$E_{rot} = J(J+1) * 7.06 * 10^{-22} \text{ J}.$$

This suggests a somewhat lower activation temperature of 102 K. The quadratic fit of the minimum of Figure 8 gives a spring constant of $k = 0.321$ so the vibrational energy levels are subject to the correction $\sqrt{0.321/0.360}$ to obtain

$$E_{rot} = 8.15 * 10^{-20} (n + \frac{1}{2}) \text{ J}.$$

	$R(\text{\AA})$	$\langle H \rangle_{min}$	$\tilde{\nu}(\text{cm}^{-1})$
Experiment	0.742	-1.17	2170
ψ_T	0.762	-1.14	2080.6
ϕ_T	0.878	-1.00	2070

TABLE I.

The activation temperature is again lowered to $T = 2950$ K while the ground state frequency is actually improved relative to experiment to $\tilde{\nu} = 2070 \text{ cm}^{-1}$.

V. DISCUSSION

For the hydrogen atom, we attempted to directly compute the equilibrium bond length and establish a good estimate for the ground state energy by minimizing $\langle H \rangle$. Since our procedure for arriving at both was dependent on the choice of trial wavefunction, we employed two different choices in order to compare results. In these results summarized in the first three columns of Table V, the spatially symmetric combination of hydrogen ground state wavefunctions ψ_T clearly matched experiment better. This comes as no surprise, since it is essentially saying that the form of the ground state does not change much as two hydrogen atoms become one hydrogen molecule.

However, clearly something has to change in the molecular case. One area for future study would be to remove the spherical symmetry from the trial wavefunctions. The molecule introduces a preferred direction, that of \mathbf{R} , and the naive picture of a covalent bond is that the electron orbitals will overlap in the space between the atoms, so there is motivation for bringing in angular dependence.

Another thing that could change in the molecular case is the expected distance of the electrons from the nuclei. While we did not calculate $\langle r \rangle$, a gives us a good idea of the characteristic distance of the electrons in their spherically shaped orbitals. It was surprising that at the R which minimized the local energy, the minimum along the a axis was achieved at $a = 0.9a_0$, indicating a tighter distribution of electrons than atomic hydrogen. This seems counterintuitive since the nuclear charge has not increased, and there is electron-electron repulsion. However, these are simplistic arguments which could certainly be overruled by deeper physics.

One last interesting quantity can be found from our direct results as a final check on the accuracy of our local energy minimization. This is the disassociation energy, or the energy required to break the molecule into two separate atoms. This reduces the problem to moving the two atoms away and so we can calculate

$$E_{dis} = E(R \rightarrow \infty) - E(R_{bond}).$$

Interpolating from Figure 7 we obtain that E_{dis} is roughly 0.06 in our unit system or 1.6 eV using the trial wavefunction ψ_T . Using ϕ_T and Figure 8, we obtain 0.15

or 4.1 eV. The latter is the better value given the experimental disassociation energy of H_2 , 4.75 eV [1]. Most likely, the great discrepancy of E_{dis} for ψ_T is due to the fact that we only calculated $\langle H \rangle$ as far out as $R = 2a_0$ in Figure 7, which is obviously not a good approximation of $R = \infty$.

Appendix A: Extension to the Deuterium Molecule

A simple extension of the physics explored in this paper can be made to the deuterium molecule, D_2 . Quantum mechanically, this system is still described by Equation 4. The only difference is that the additional neutron in each nucleus means that the reduced mass (which was simply $\frac{1}{2}m_p$ before) is now

$$\mu = \frac{2m_p * 2m_p}{2m_p + 2m_p} = m_p.$$

Since the hydrogen atom trial wavefunction ψ_T gave results that best agreed with experiment, we will apply the deuterium modifications to those values. The new

reduced mass means that the rotational spectrum is

$$E_{rot} = \frac{J(J+1)(1.05 * 10^{-34})^2}{2 * 1830 * 9.11 * 10^{-31}(1.44 * 5.29 * 10^{-11})^2}$$

$$= J(J+1) * 5.70 * 10^{-22} \text{ J}.$$

Then the activation temperature of $T = 82.6$ K is half what it was for diatomic hydrogen. The vibrational energy levels are governed by the angular frequency

$$\omega = \sqrt{k/\mu} = \sqrt{0.360/1830} = 0.0140.$$

After converting in the same way as in Section IV A 2, we can arrive at an expression for the vibrational modes of D_2 :

$$E_{vib} = 6.10 * 10^{-20} (n + \frac{1}{2}) \text{ J}.$$

As before, we are interested in the activation temperature and the ground state frequency, which we determine to be

$$T = \frac{1}{k_B} * 6.10 * 10^{-20} (\frac{1}{2}) = 2210 \text{ K},$$

$$\tilde{\nu} = \frac{1}{hc} * 6.10 * 10^{-20} (\frac{1}{2}) = 1530 \text{ cm}^{-1}.$$

The latter quantity matches the one reported by the literature, $\tilde{\nu} = 1523 \text{ cm}^{-1}$ [5].

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