Calculation of the Ground State of ^{4}He

via the **Variational Monte Carlo Method**

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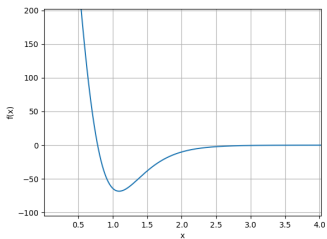
Goal: Calculate the ground state of the ^{4}He.

We will consider the Afnan-Tang S3 interaction:

$$V(r_1, r_2, r_3, r_4) = \sum_{i<j} \Big[1000\, e^{-3 r_{ij}^2} - 163.35\, e^{-1.05 r_{ij}^2} - \\ - 21.5\, e^{-0.6 r_{ij}^2} - 83\, e^{-0.8 r_{ij}^2} - 11.5\, e^{-0.4 r_{ij}^2} \Big]$$



Trial wave function:

$$\psi_T(r_1, r_2, r_3, r_4) = \prod_{i<j} \Big[e^{-\gamma r_{ij}^2} + \alpha\, e^{-\beta r_{ij}^2} \Big]$$

Variational Principle and Local Energy

$$\langle H \rangle = \frac{\int \psi^* H \psi \, d\mathbf{R}}{\int \psi^* \psi \, d\mathbf{R}} \geq E_0 \tag{1}$$

Local energy:

$$E_L(\mathbf{R}) = \frac{H\psi(\mathbf{R})}{\psi(\mathbf{R})}$$

$$\langle H \rangle = \frac{\int d\mathbf{R} \, \psi_T^*(\mathbf{R}) H \psi_T(\mathbf{R})}{\int d\mathbf{R} \, |\psi_T(\mathbf{R})|^2} = \frac{\int d\mathbf{R} \, \psi_T^*(\mathbf{R}) \psi_T(\mathbf{R}) \psi_T^{-1}(\mathbf{R}) H \psi_T(\mathbf{R})}{\int d\mathbf{R} \, |\psi_T(\mathbf{R})|^2}$$

$$= \int d\mathbf{R} \frac{|\psi_T(\mathbf{R})|^2}{\int d\mathbf{R} \, |\psi_T(\mathbf{R})|^2} E_L(\mathbf{R}) \approx \frac{1}{M} \sum_{i=1}^{M} E_L(\mathbf{R}_i) \tag{2}$$

$$E_V = \frac{1}{M}\sum_{k=1}^{M} E_L \tag{3}$$

E_L is a random variable, taking different values in different sampling. The central limit theorem states that if E_L are independent variables, then in the large M limit the probability distribution of the random variables E_L converges to a gaussian of expectation value $E[E_L] = E_V$ and variance $[E_V]$

$$\begin{cases} E_V = E[E_L] \\ Var[E_V] = \dfrac{Var[E_L]}{M} \end{cases}$$

E_v is an estimator of the energy of the system.

$$P[E_V]_{M\to\infty} = \frac{1}{\sqrt{2\pi\sigma_{E_V}}} e^{-\frac{(E_V-\langle H\rangle)^2}{\sigma^2_{E_V}}}$$

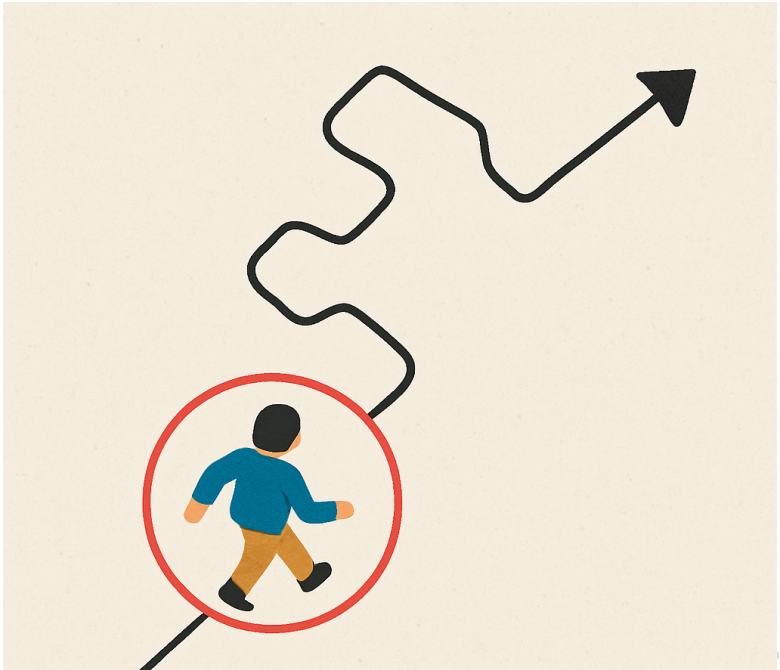
How we can sample from a $|\psi|^2$ *distribution*?

Metropolis algorithm:

$$A(\mathbf{R} \leftarrow \mathbf{R}') = \min\left(\frac{|\psi(\mathbf{R}')|^2}{|\psi(\mathbf{R})|^2}, 1\right)$$

In the Metropolis-Hastings algorithm [12, 13], one realizes a Markov chain with the following random walk. Starting from a point Ri, a new point Rf is determined in two steps:

- a temporary point R' f is proposed from a uniform distribution
- If the probability $|\psi(\mathbf{R}')|^2$ is greater than $|\psi(\mathbf{R})|^2$, the transition is accepted
- If the probability $|\psi(\mathbf{R}')|^2$ is smaller than $|\psi(\mathbf{R})|^2$, the transition is accepted with probability $\frac{|\psi(\mathbf{R}')|^2}{|\psi((\mathbf{R}))|^2}$
- In case of rejection, the walker stays in the old state $\mathbf{R}$



Python code

```
# Step 1: Initialize walker positions
X_Old = 10 * StepSize * ((np.random.rand(NA, 3) - 0.5))
```

```
# Step 2: Calculate wave function and initialize energy variables
wave_Old = wave_function(X_Old, alpha, beta, gamma)
energy = 0
energy2 = 0
```

```
# Step 3: Loop of moves and loop of steps
for MCcycle in range(NumberMCcycles):
    for _ in range(Ntherms): # Thermalization steps
```

Python code

```
#step 4: Metropolis algorithm
X_new[i] += StepSize * (np.random.rand(3) - 0.5)
wave_New = wave_function(X_new, alpha, beta, gamma)
log_ratio = 2 * ( np.log(abs(wave_New)) - np.log(abs(wave_Old)) )
if log_ratio >= np.log(np.random.rand()):
    X_Old[i] = X_new[i]
    wave_Old = wave_New
```

```
# Step 5: energy sampling
elocal = local_energy(wave_Old, X_Old, alpha, beta, gamma)
energy += elocal
energy2 += elocal ** 2
```

Python code

```
#Step 6: mean energy
mean_energy = energy / NumberMCcycles
mean_energy2 = energy2 / NumberMCcycles
error = sqrt((mean_energy2 - mean_energy ** 2) / NumberMCcycles)
```

```
#Step 7: repeat the process for different alpha, beta, gamma
for ia in range(MaxVariation):
    for jb in range(MaxVariation):
        for kc in range(MaxVariation):
            ...
            ...
            ...
            alpha += 0.5
            beta += 0.35
            gamma += 0.012
```

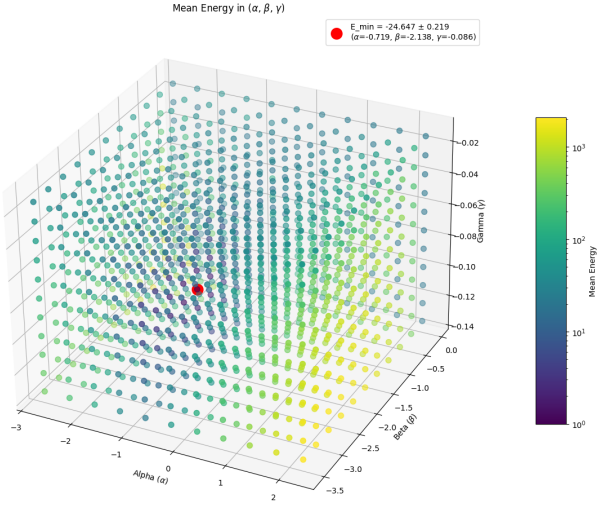
Remark

The main hypothesis underlying the Central Limit Theorem is that data used to construct the averages are sampled independently. In the case of the computation of an integral by the Metropolis Hastings method this requirement is not satisfied by construction.
The error associated in case of correlation is $\Delta I \approx \sqrt{\frac{\sigma(E_L)^2}{N-1}\bar{\tau}}$, where $\bar{\tau}$ is the autocorrelation length.

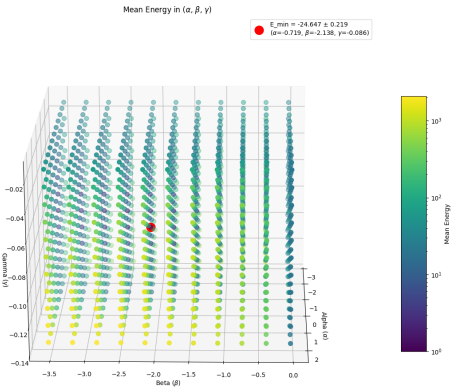
- We choose Δ in order to have an acceptance rate $\approx 60\%$ (in our case $\Delta = 2$)
- Thermalisation: Starting at a given state s_i, we proceed carrying out a given number n of intermediate steps, but we only count or collect the state s_{i+n} after n steps, and so on. In other words, "$n-1$ intermediate steps are discarded.

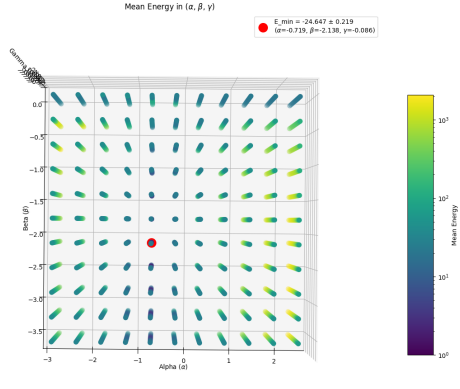
```
for _ in range(Ntherms): # Thermalization steps
```

Result

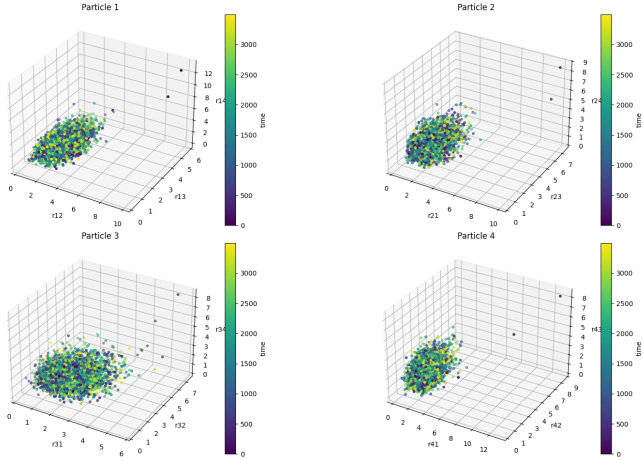


(11 x 11 x 11) values of (α, β, γ).
20'000 samples for each configuration



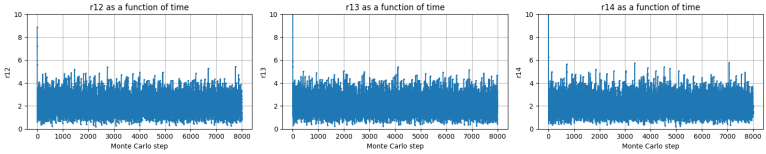


ground state energy: -24.6 ±0.2. $(\alpha, \beta, \gamma) = (0.7191, 2.13796, 0.08597)$

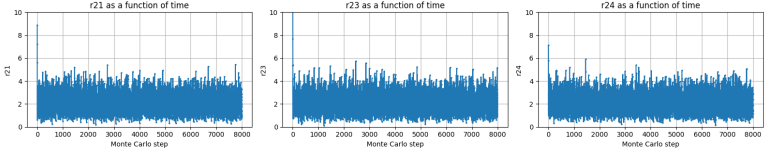


space distribution

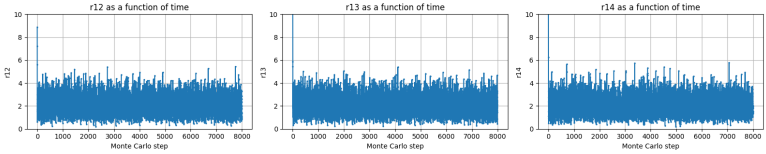
Particle 1: r_ij coordinates as a function of time



Particle 2: r_ij coordinates as a function of time



Particle 1: r_ij coordinates as a function of time



Particle 4: r_ij coordinates as a function of time