

# VARIATIONAL MONTE CARLO FOR SUPERFLUID $^4\text{He}$

Matteo Bettanin, Francesco Musso, Matteo Scandola

November 29, 2021

## Introduction

For temperatures below approximately 2.17 K  $^4\text{He}$  is in a superfluid state. Superfluid Helium can be treated as  $N$  point-like particles in the ground state of the following Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{i<j}^N V(r_{ij}) \quad (1)$$

in which the potential is the 6-12 Lennard-Jones potential

$$V(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (2)$$

with  $\varepsilon = 10.22 \text{ K}$  and  $\sigma = 0.2556 \text{ nm}$ .

Our aim in this project is to find the ground state energy per atom. This will be achieved through a Variational Monte Carlo (VMC) procedure. A Variational Monte Carlo (VMC) procedure is an implementation of the variational theorem which exploit the Monte Carlo technique to evaluate the energy functional for the trial wave function at different values of the variational parameters.

Since the system is strongly correlated the trial wave function we choose is a Bill-Jastrow type wave function for bosons, with a single variational parameter  $b$ .

$$\Psi_T(\mathbf{r}_1, \dots, \mathbf{r}_N) = \exp \left[ -\frac{1}{2} \sum_{i<j}^N \left( \frac{b}{r_{ij}} \right)^5 \right] \quad (3)$$

The chosen function respect the symmetries of the system and fulfill the following requirement

$$\frac{\hat{H}f(r_{ij})}{f(r_{ij})} < \infty \quad (4)$$

commonly called *cusp condition*, which guarantees that the wave function is small when the potential is large.

We simulates the bulk of  $^4\text{He}$  using periodic boundary conditions on a system of 32 particles. The validity of this kind of approximation will be checked later.

The work from *McMilann*<sup>1</sup> is used as reference for the results, since our work it's basically a replica of his.

## 1 Typical units of the system

In order to simplify the computation we consider a unit system in which  $\varepsilon$  and  $\sigma$  are equal to one. The potential becomes

$$V(r) = 4 \left[ \left( \frac{1}{r} \right)^{12} - \left( \frac{1}{r} \right)^6 \right] \quad (5)$$

and the kinetic energy constant  $\hbar^2/2m$  becomes:

$$\frac{\hbar^2}{2m} = \frac{\hbar^2}{2m} \cdot \frac{1}{\varepsilon \sigma^2} [\varepsilon][\sigma^2] = 0.091 [\varepsilon][\sigma^2] \quad (6)$$

<sup>1</sup><https://doi.org/10.1103/PhysRev.138.A442>

## 2 Initial configuration

The starting configuration of any of the following Monte Carlo calculations will be equal to 8 unitary cells of a face centred cubic lattice each one containing 4 atoms. The four atoms in a cell have coordinates  $(0,0,0)$ ,  $(a/2,a/2,0)$ ,  $(0,a/2,a/2)$ ,  $(a/2,0,a/2)$ , where  $a$  is the lattice parameter.

The lattice parameter is chosen in order to accommodate the 32 particles in the 8 cells at a given density, then  $a$  will be equal to  $L/2$ , where  $L$  is the side of the entire box, obtained as  $L = (32/\rho)^{1/3}$

To obtain the starting configuration we implement a routine which given the number  $N$  and  $a$  the lattice parameter return an  $N \times 3$  array with the Cartesian coordinates of every atom.

The result for  $N = 32$  at the experimental saturation density of  $^4\text{He}$   $\rho_0^{\text{exp}} = 21.85 \text{ nm}^{-3}$  is shown in figure 2.

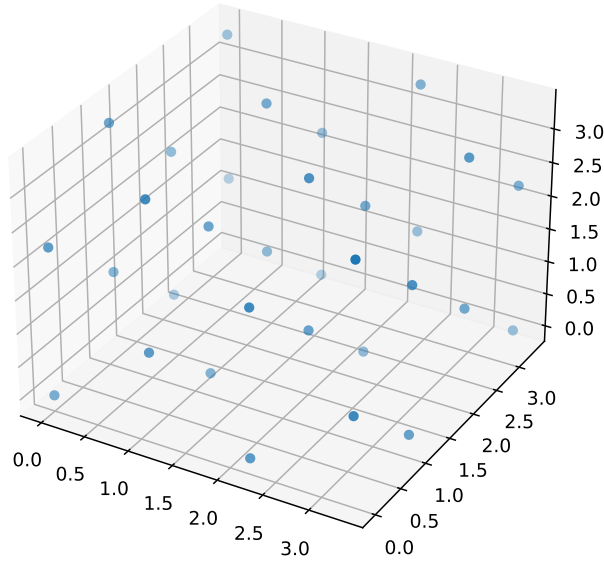


Figure 1: Fcc lattice for 32 particles

### 2.1 PBC and cutoff distance

Since our aim is to simulate the properties of the bulk of  $^4\text{He}$ , we treat the system as an infinite periodic system. To do so we implement Periodic Boundary Conditions (PBC). The box is replicated to form an infinite lattice of equal boxes. In the simulation every time a particle is displaced in a way that would make it exit from its box, it is reintroduced at the opposite side, as if its image in the nearest box entered the box.

In order to comply with the minimum image convention we set a cutoff at  $r_c = L/2$ , setting to zero any interaction energy between particles further away than  $r_c$ . This caveat introduces some errors in the calculation which neglect long-range interactions, and in the general for small number of particle, like in our case, it is sensible to check how much the symmetries of the periodic lattice influence the system by simulating the system with more particles.

### 3 Monte Carlo procedure

Monte Carlo methods are a class of stochastic algorithm used to integrate functions that have no easy analytical solution. The idea beneath this method is that by treating the integration variable as a random variable, the integral value can be approximated by the average value of the integrand calculated on different samples of the random variable. This method can be applied to our problem since we want to calculate the energy of the system, which is nothing but an integral over the coordinates of the particles in our system. The various possible configurations are the random variable we integrate upon, with the probability distribution given by the squared wave function.

To compute the variational integrals we will use a *Markov-chain-Monte-Carlo* method, such as the Metropolis-Hastings algorithm. This algorithm allows us to sample the random variable according to their probability density, on which the integral value will be estimated.

In our case the algorithm works in the following way, starting from the fcc configuration:

- The value of the wave function  $\Psi_T$  on the configuration is
- A displacement of one or more atoms of the system is proposed
- The value of the wave function  $\Psi_T^{\text{new}}$  on the proposed configuration is computed
- The acceptance ratio is calculated:  $\kappa = \frac{\Psi_T^{\text{new}}}{\Psi_T}$
- if  $\kappa > 1$  the displacement is accepted and the configuration becomes the proposed one.
- if  $\kappa < 1$  we extract a random number  $\eta \in [0, 1]$  and if  $\kappa > \eta$  we still accept the displacement, else we refuse the displacement and keep our old configuration.

By iterating this process a chain of configuration can be created, which after some steps will recreate the probability distribution of the random variable. In our case this means allowing the system to reach equilibrium, then discarding the first values of the chain: how many will be discussed in the following.

The central limit theorem, on which the Monte Carlo estimation of integral is based, states that the samples of the random variable must be independent, which is definitely not the case for a Markov chain. In order to address this problem we estimate the *autocorrelation coefficient* as

$$c(E)_\tau = \frac{\langle E(X_i)E(X_{i+\tau}) \rangle - \langle E \rangle^2}{\langle E^2 \rangle - \langle E \rangle^2} \quad (7)$$

which measures the correlation between the energy value at the Markov chain step  $i$  and the step  $i + \tau$ , and usually goes like  $e^{-\frac{\tau}{\bar{\tau}}}$ . By fitting the autocorrelation coefficient with the exponential, we can obtain the value of  $\bar{\tau}$ , called *autocorrelation time*, which gives an estimate of the distance of number of steps between two independent configurations. We can then calculate the value of the energy every  $\bar{\tau}$  steps of the Markov chain and the error on the integral value will simply be the standard deviation of the energy values, divided by the squared root of the number of samples.

In order to lower the correlation time, the ratio between the accepted Monte Carlo proposals and the total steps must be between 30% and 60%. The value that controls this ratio is usually referred as  $\Delta$  and represents the maximum possible displacement of an atom in a proposal. By taking a very small value of  $\Delta$  all new proposal will be accepted with little gain of new information at every step which will result in a big autocorrelation time. Vice versa if  $\Delta$  is too big, very few steps will be accepted and again the autocorrelation time will be big, since the chain is stuck always on the same configuration.

To avoid this behaviour in the first  $10k$ , the equilibration phase, we implemented an algorithm to update the value of  $\Delta$  based on the ratio of accepted proposals every  $1k$  steps. After the equilibration phase, we compute

energy values on  $10k$  steps, which are used to obtain the autocorrelation time. In the end we calculate and save 50k values of the energy, computed every  $\bar{\tau}$  steps, effectively computing  $50000\bar{\tau}$  steps of the Markov chain. These values are used to estimate the integral.

### 3.1 Local energy estimation

As said before we need to evaluate the energy functional for the trial wave function

$$E[\Psi_T] = \int dR |\Psi(r_1 \dots r_N)|^2 \frac{H\Psi(r_1 \dots r_N)}{\Psi(r_1 \dots r_N)} = -\frac{\hbar^2}{2m} \int dR |\Psi(r_1 \dots r_N)|^2 E_L \quad (8)$$

where the *local energy* has been introduced as

$$E_L = \frac{H\Psi(r_1 \dots r_N)}{\Psi(r_1 \dots r_N)} = \underbrace{-\frac{\hbar^2}{2m} \sum_{\ell=1}^N \frac{\nabla_{\ell}^2 \Psi(r_1 \dots r_N)}{\Psi(r_1 \dots r_N)}}_{T_L} + \underbrace{\sum_{i < j}^N V(r_{ij})}_V \quad (9)$$

The local kinetic energy  $T_L$  will be

$$\begin{aligned} T_L &= -\frac{\hbar^2}{2m} \sum_{\ell} \frac{\nabla_{\ell}^2 \Psi(r_1 \dots r_N)}{\Psi(r_1 \dots r_N)} = -\frac{\hbar^2}{2m} \sum_{\ell} \left[ -\frac{1}{2} \nabla_{\ell}^2 \sum_{i < j} u(r_{ij}) + \frac{1}{4} \left( \nabla_{\ell} \sum_{i < j} u(r_{ij}) \right)^2 \right] = \\ &= -\frac{\hbar^2}{2m} \sum_{\ell} \left[ -\frac{1}{2} \sum_{i \neq \ell} \frac{d^2 u(r_{i\ell})}{dr_{i\ell}^2} + \frac{2}{r_{i\ell}} \frac{du(r_{i\ell})}{dr_{i\ell}} + \frac{1}{4} \left( \sum_{i \neq \ell} \frac{du(r_{i\ell})}{dr_{i\ell}} \frac{\mathbf{r}_{i\ell}}{r_{i\ell}} \right)^2 \right] \\ &= -\frac{\hbar^2}{2m} \sum_{\ell} \left[ -\frac{1}{2} \sum_{i \neq \ell} \frac{20b^5}{r_{i\ell}^7} + \frac{1}{4} \left( \sum_{i \neq \ell} \frac{5b^5}{r_{i\ell}^7} \mathbf{r}_{i\ell} \right)^2 \right] \end{aligned} \quad (10)$$

Note that since the kinetic energy is the integral of the local kinetic energy another valid local estimator of the kinetic energy can be the Jackson-Feenberg one<sup>2</sup>:

$$\begin{aligned} T_L^{JF} &= -\frac{\hbar^2}{4m} \left[ \sum_{\ell} \frac{\nabla_{\ell}^2 \Psi(r_1 \dots r_N)}{\Psi(r_1 \dots r_N)} - \left| \frac{\nabla_{\ell} \Psi(r_1 \dots r_N)}{\Psi(r_1 \dots r_N)} \right|^2 \right] = \frac{\hbar^2}{8m} \sum_{i \neq \ell} \nabla_{\ell}^2 u(r_{i\ell}) \\ &= \frac{\hbar^2}{8m} \sum_{\ell} \sum_{i \neq \ell} \frac{d^2 u(r_{i\ell})}{dr_{i\ell}^2} + \frac{2}{r_{i\ell}} \frac{du(r_{i\ell})}{dr_{i\ell}} = \frac{\hbar^2}{8m} \sum_{\ell} \sum_{i \neq \ell} \frac{20b^5}{r_{i\ell}^7} \end{aligned} \quad (11)$$

The values of the two local energy estimator may differ for the same configuration, but the integral value must be the same since they represents the same integral. This consideration will be useful to check the correctness of our implementation.

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<sup>2</sup> $T = \int \Psi^* \nabla^2 \Psi = - \int |\nabla \Psi|^2 \implies T = 1/2 \int \Psi^* \nabla^2 \Psi - |\nabla \Psi|^2$

## 4 Variational procedure at the experimental saturation density

We implement the variational procedure by simply repeating the integral evaluation for different values of  $b$ , close to 1.17, which should be near the best value of  $b$ .

The result of our variational calculation for the experimental saturation density  $\rho_0 = 21.85 \text{ nm}^{-3}$  are reported in figure 4.

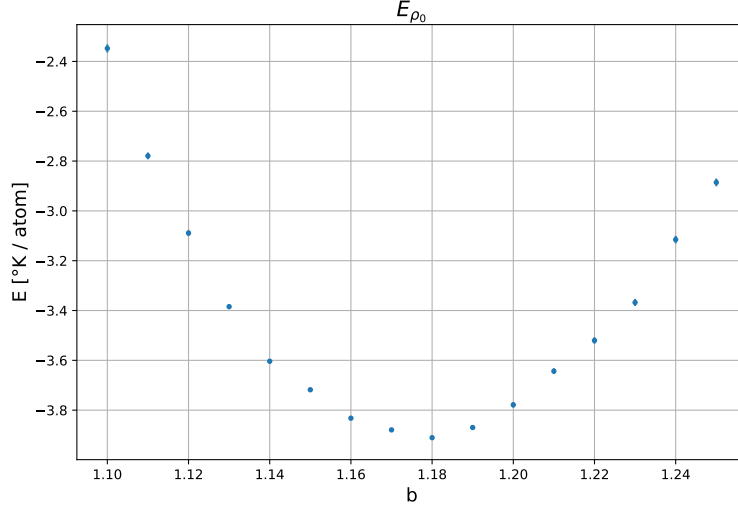


Figure 2: Variational calculation on parameter  $b$  of the wave function at  $\rho_0$

We obtain the minimum at  $b = 1.18$  with the following results:

- $E = (-3.91 \pm 0.01) \text{ K/atom}$
- $T = (13.27 \pm 0.02) \text{ K/atom}$
- $V = (-17.19 \pm 0.02) \text{ K/atom}$
- $T_{JF} = (13.810 \pm 0.007) \text{ K/atom}$

In order to check the correctness of our implementation we plot in the following figures the energy values of 1000 steps of the integral evaluation for  $b = 1.18$ . The fit for the autocorrelation coefficient it's done by approximating the integral over  $c(E)_p \tau$ , which would give  $\bar{\tau}$  as result, with the sum of the first 250 values of  $c(E)_\tau$ .

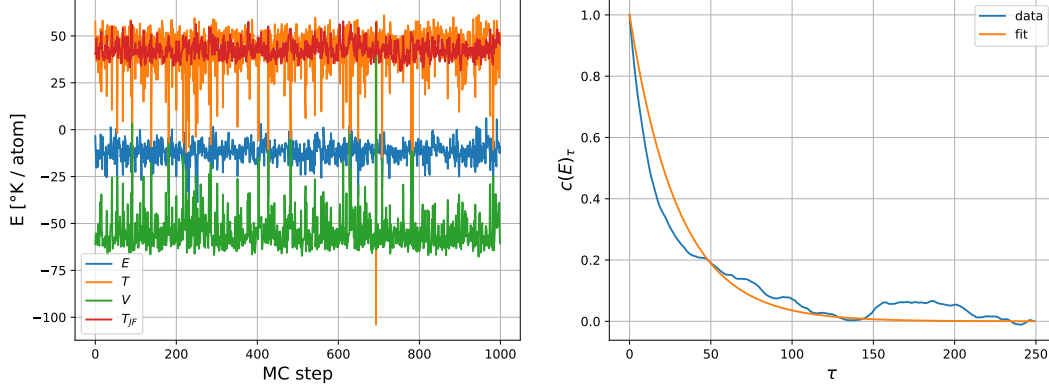


Figure 3: Example of energy values at every step and autocorrelation coefficient for  $b = 1.18$

As we can see in the figure the *Jackson-Feenberg* estimator for the kinetic energy has a much lower variance, but it is not anti-correlated to the potential estimator, while  $T$  it is. If the energy was to be computed using the *Jackson-Feenberg*, as it is in the McMillan work, its value would fluctuate much more, resulting in a bigger error on the integral.

We said before that the average value of  $T$  and  $T_{JF}$  should be the same, since they represent the same quantity. This is in fact true, but in this case we notice a discrepancy between the two value. We attribute this discrepancy to the fact that the interaction between particles is truncated at the cutoff radius  $r_c = L/2$ , since the relation  $\langle T \rangle = \langle T_{JF} \rangle$  holds only when the integration is carried out on all space, which it is technically different from what we have done here by truncating the interaction at  $r_c$ . In the next section we will try to account for the error caused by the truncation.

#### 4.1 Long Range Correction

By comparing our result with the McMillan ones, we notice they are quite different, with ours being much higher. This is due to the truncation of the interaction between particles at  $r_c = L/2$ . In our system at  $\rho_0$  the box side  $L \simeq 4.4\sigma$  and just by calculating

$$V(r_c) = -0.33\text{K} \quad (12)$$

we can note that the interaction left off will give a considerable contribution to the energy.

In order to account for the left off interaction we use the so-called *long range correction* which consists in taking the pair distribution function  $g(\mathbf{r})$  equal to 1 in equation 11 of McMillan reference article for  $r > r_c$ . Then by integrating we get the following correction

$$E_{LRC}(\rho, b) = \frac{\hbar^2}{2m} \pi \rho \frac{5b^5}{r_c^4} + \frac{8}{3} \pi \rho \left( \frac{1}{3r_c^9} - \frac{1}{r_c^3} \right) \quad (13)$$

where the first term of the sum is due to the kinetic interaction, while the second one to the potential.

So, in order to make a quantitative comparison with the reference article we add the long range correction to the variational calculation. Since the formula used to calculate the long range correction is derived from the *Jackson-Feenberg* kinetic energy formula, our new energy values will be

$$E = T_{JF} + V + E_{LRC} \quad (14)$$

which are plot in figure 4.1.

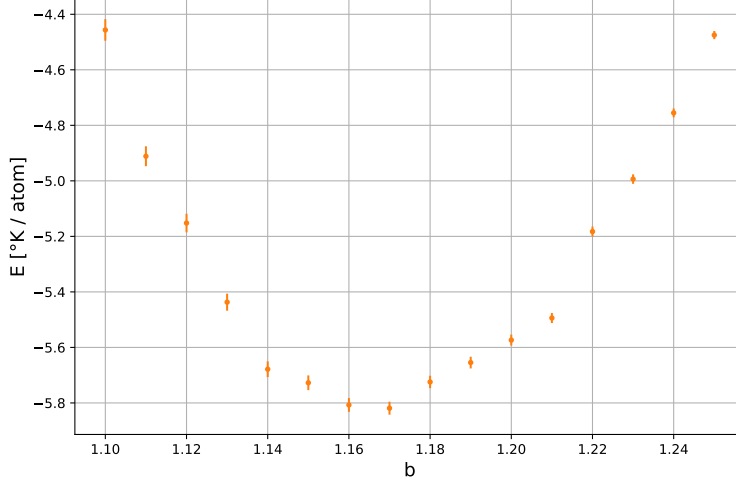


Figure 4: Variational calculation  $\rho_0$  with the long range correction

Our new estimate for the ground state energy (with  $b = 1.17$ ) becomes

$$E = (-5.81 \pm 0.02) \text{ K/atom} \quad (15)$$

which is compatible with the McMillan's result at  $\rho_0$  of  $E = (-5.6 \pm 0.1) \text{ K/atom}$

## 4.2 Periodic boundary condition effects

As said before, in order to check the effects of the periodic boundary conditions we perform the integration for  $N = 108$ , at  $b = 1.17$ . Again the initial configuration is fcc lattice, of side  $L \simeq 6.6\sigma$  at  $\rho_0$ .

The major effect of increasing the number of particles in our case is, by having a bigger box, to have a larger cutoff radius, which means a better estimation of the energy via the Monte Carlo method and even a better approximation in the long range correction, since in the region  $r > L/2$  the pair distribution function  $g(\mathbf{r})$  will be closer to 1.

We obtain the following values (without the the long range correction):

- $E = (-5.010 \pm 0.005) \text{ K/atom}$
- $T = (13.81 \pm 0.01) \text{ K/atom}$
- $V = (-18.9 \pm 0.1) \text{ K/atom}$
- $T_{JF} = (13.900 \pm 0.005) \text{ K/atom}$

These results verify most of the consideration we made before: the difference between the two estimators for the kinetic energy tends to vanish with the increase of the cutoff radius and the total energy is considerably lower. By including the long range correction we obtain

$$E = (-5.76 \pm 0.01) \text{ K/atom} \quad (16)$$

which is again compatible with the McMillan's result and even compatible with the previous result with  $N = 32$ . These confirm the validity of the simulation of the bulk with the periodic boundary condition.

## 5 Theoretical saturation density

Finally we repeat the VMC procedure at different densities, in order to establish the theoretical saturation density for the model.

We perform the variational calculation for different values of  $b$  at different densities with  $0.75 \leq \rho/\rho_0 \leq 1$ . We report our results in figure 5

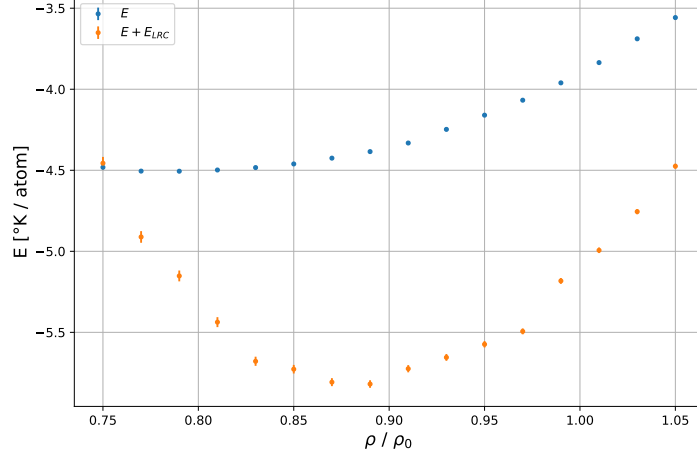


Figure 5: Energy (with or without long range correction) as function of the density

We obtain the minimum of  $E = (-5.91 \pm 0.02)$  K/atom, with our saturation density equal to  $\rho/\rho_0 = 0.89 \pm 0.02$ , once again compatible with the values of the reference of  $E = (-5.9 \pm 0.1)$  K/atom at  $\rho/\rho_0 = 0.89 \pm 0.01$ .

We note that the effect of the long range correction is, once again, decisive. The omission of such a correction would have lead to completely wrong conclusions about the the theoretical saturation density. Once again better results could be obtained by increasing the number of particles, but at a large computational cost compared to the gained accuracy.