1 Introduction

Especially in the branch of statistical or many-particle physics, high-dimensional integrals occur in a large variety. With standard methods like the trapezoidal rule, Simpson's rule or Gaussian quadrature the numerical calculations are getting more and more expensive with increasing number of particles and therefore higher dimensions of the integrals. For this purpose, the so called Monte-Carlo (MC) integration has been developed which uses statistical methods for evaluating this high-dimensional integrals.

The MC-method for solving integrals and its application to many-particle quantum physics is described in the following paper. The variational Monte Carlo (VMC) method will be used to approximate the ground state of an interaction many-body system consisting of identical bosons.

2 Theory

2.1 Monte-Carlo integration

For the numerical treatment of integrals, literature provides a huge variety of distinct methods like trapezoidal rules, or more sophisticated Gaussian quadrature rules. In all cases the integral is replaced by a sum, where a function is evaluated on particular points (sampling points) determined by the function itself. Gaussian quadrature approximates a definite integral as a weighted sum [1], i.e.

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{i=1}^{N} w_i f(x_i)\ . \tag{2.1}$$

In order to evaluate the integral with an appropriate accuracy, the number of sampling points N has to be increased. This leads to a sensitive dependence on the dimensionality d of the integral, because if one discretizes every integration dimesion with N points, the number of sampling points yields N^d. For low - dimensional integrals ($d = 1, \ldots, \sim 7$) the computational costs may be accepted on modern computers.

However, for high dimensional problems as they appear for example in statistical, or many-particle physics this type of integration is much too expensive. By the usage of statistics, a non-deterministic approach can be used, which is called *Monte-Carlo* (MC)

integration. A highly dimensional integral is approximated by

$$\int_\Omega f(x)\,\mathrm{d}x = \frac{1}{N}\sum_{i=1}^{N} f(\bar{x}_i)\ , \tag{2.2}$$

where V denotes the m-dimensional integration volume. The bar indicates the evaluation of the function f at random points, i.e. $\bar{x}_i \in U_\Omega$ where U denotes a uniform distribution in the integration space Ω. It can be shown that the estimated error of MC-integration is of the order $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$. Therefore, for a high dimensional integration space, the number of random sampling points are much lower to reach a desired accuracy as for the integration with conventional numerical methods.

The problem of high dimensional numerical integration is hence reduced in order to find a proper probability function $P(x)$ for the extraction of random sampling points. Depending on the underlying physical system such distributions can be found with the *Metropolis-Hastings* algorithm.

2.2 Application to quantum theory

In the quantum mechanical treatment of many-particle physics the Hamiltonian introduced for finding a solution of Schrödinger's equation can be written in a general form as

$$\mathcal{H} = -\sum_{i=1}^{N}\frac{\hbar^2}{2m}\nabla^2 + \sum_{i=1}^{N} u(\boldsymbol{r}_i) + \sum_{i<j}^{N} v(\boldsymbol{r}_i - \boldsymbol{r}_j)\ , \tag{2.3}$$

where the first term describes the kinetic energy of the i-th particle, the second term is an external potential, and the third term denotes two center interactions. In this case, higher order interactions has been neglected.

In order to find a ground state energy the variational principle of Ritz is used. Considering Schrödingers equation $\mathcal{H}\,|\psi\rangle = E_0\,|\psi\rangle$ [2] it follows, that the ground state energy is given by minimization of

$$\langle\mathcal{H}\rangle = \frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0\ , \tag{2.4}$$

where equality is reached for $\psi = \psi_0$ (the groundstate).

Since the dimensionality of the Hamiltonian given by Eq. 2.3 is of the order of $d = 3N$, the expectation value according to Eq. 2.4 yields a $3N$ dimensional integral. This

motivates the usage of MC-integration.

2.3 Variational Monte Carlo

The main idea of variational Monte Carlo (VMC) is to find a sophisticated ansatz for the wavefunction ψ which is called *trial-wavefunction* and is denoted as ψ_T. Such ansatz can be written as a product of two-center functions which has been introduced first by Jastrow and Feenberg, i.e.

$$\psi_T = \prod_{i<j}^{N} f(\boldsymbol{r}_i - \boldsymbol{r}_j) \ . \tag{2.5}$$

This function may depend on a set of optimization parameters $\{\alpha_m\}$. The particular values of each α_m can be found by minimizing the total energy according to Eq. 2.4 . Therefore, the trial energy can be written as

$$\begin{aligned} E_T &= \frac{\langle\psi_T|\mathcal{H}|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} = \frac{\int \mathrm{d}\boldsymbol{R}\,\psi_T^*\mathcal{H}\psi_T}{\int \mathrm{d}\boldsymbol{R}\,\psi_T^*\psi_T} \\ &= \frac{\int \mathrm{d}\boldsymbol{R}\,|\psi_T|^2\,\frac{1}{\psi_T}\mathcal{H}\psi_T}{\int \mathrm{d}\boldsymbol{R}\,|\psi_T|^2}, \end{aligned}$$

where $\boldsymbol{R}$ denotes a $3N$ dimensional vector of all particles in $d = 3$ spatial dimensions. By introducing the local energy

$$E_l = \frac{1}{\psi_T}\mathcal{H}\psi_T \ , \tag{2.6}$$

the trial energy can be written as

$$E_T = \int \mathrm{d}\boldsymbol{R}\,\Pi(\boldsymbol{R})E_l(\boldsymbol{R}) \ , \tag{2.7}$$

where the probability distribution $\Pi(\boldsymbol{R}) = |\psi_T|^2$ has been defined and will be used as the importance sampling distribution function in the Metropolis algorithm.

The integral given in Eq. 2.7 can be solved by MC integration, i.e.

$$E_T = \frac{1}{M}\sum_{i=1}^{M} E_l(\boldsymbol{R}_i) \qquad \boldsymbol{R}_i \in |\psi_T|^2 \ . \tag{2.8}$$

For the evaluation of random coordinate moves, the Metropolis algorithm is used:

1. Considering a system of N particles: choose randomly one particle with index i and perform a random move of all coordinates m to obtain $r'_{i,m} = r_{i,m} + \Delta(\xi_m - 1/2)$ where $\xi_m \in U[0,1]$ and Δ is a constant that determines the size of the shift.
2. Calculate the ratio $a = \left|\frac{\psi_T(\boldsymbol{R}')}{\psi_T(\boldsymbol{R})}\right|^2$ and only accept the new coordinates with probability $A = \min[1, a]$
3. Perform the MC summation for every p-th step, i.e. $E_{p+1} = E_p + E_l(\boldsymbol{R}_p)$
4. Repeat the steps 1 – 3 as long as a sufficient number of P steps is reached.
5. The final energy value equals $E_T = \frac{1}{P}\sum_p E_p$. Furthermore error bars for the quantity E_T can be calculated.

Note that an analytical expression for E_l has to be found by evaluating $\mathcal{H}\psi_T$ for a given ansatz ψ_T. Since the trial wavefunction ψ_T is in general a function of optimization parameters α_m, the algorithm has to be repeated for every different set of $\{\alpha_m\}$, in order to find the set of parameters $\{\alpha_m\}$ that will minimize the energy of the system.

3 Numerical implementation

In the following, the numerical implementation of the VMC method is developed in the programming language `C++`. The system under study is a strongly correlated Bose-Einstein condensate (BEC) consisting of N bosons. The generic Hamiltonian is given by Eq. 2.3 . During the implementation, two different trial wavefunctions will be considered. However, for the present implementation some assumptions will be made concerning the interaction terms in the Hamiltonian.

3.1 Particles as hard spheres

In the limit of low energies and large distances, the s-wave scattering is dominant. This can be approximated with a *hard-sphere* interaction potential

$$v(r) = \begin{cases} \infty & \text{for } r \leq a \\ 0 & \text{for } r > a \end{cases} \tag{3.1}$$

Where $a > 0$ denotes the characteristic scattering length. Furthermore, the absence of an external potential $u(r)$ has been assumed. A homogeneous system with periodic boundary conditions has been implemented, where the cubic box length is defined from $\left[-\frac{L}{2}, \frac{L}{2}\right]$. However, the box length itself has not been chosen as characteristic length scale for the simulation. Instead of this, a particle density ρ and a total number of particles N yield the box length with $L = (N/\rho)^{1/3}$. The product $a\rho^{1/3}$ can therefore be interpreted as a measure how much space the particles occupy in the simulation box.

The dimension of the system is $d = 3$ and the corresponding particle coordinates in configuration space are written in a $(N \times d)$ array. Since the boundary conditions are periodic, the nearest-image convention (NIC) has been used. A simple implementation of the NIC is shown in Listing 1. If the j-th coordinate of the i-th particle has been shifted such that the new value would exceed the size of the simulation box, it is projected back into the simulation box.

```
r = coordinates[i][j];
k = r/L + ((r >= 0.0) ? 0.5 : -0.5);
coordinatesNIC[i][j] = r - k*L;
```

Listing 1: Implementation of the NIC.

The same procedure is used for calculating the distance between two particles. The projected distance between a particle i and j is the nearest one regarding periodic boundary conditions.

3.1.1 Trial wavefunction ansatz 1:

The first trial wavefunction ψ_T is introduced as a product of the Jastrow factor

$$f_1(r) = \begin{cases} 0 & \text{for } r \leq a \\ 1 - \frac{a}{r} & \text{for } r > a \end{cases} \tag{3.2}$$

and yields

$$\psi_T(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \prod_{i<j} f(\boldsymbol{r}_i - \boldsymbol{r}_j) \; . \tag{3.3}$$

Insertion of Eq. 3.2 in Eq. 3.3 implies the abbreviation $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. Note that there is no optimization parameter α. Therefore, no variational optimization has to be performed for this Jastrow factor.

In order to ensure that periodic boundary conditions are fulfilled, the total wave function has to be 1 at $L/2$. Additionally the first and second derivative at $L/2$ has to vanish. Since the a/r term converges very slowly to zero, a smooth cutoff has been applied in the interval $r_{c1} < r < r_{c2}$. For the simulations, the values $r_{c1} = 0.7L/2$ and $r_{c2} = L/2$ are used. The function between this limits is given by a polynomial of 5th order $g(x) = Ax^5 + Bx^4 + Cx^3 + Dx^2 + Ex + F$ to get 6 free parameters to fulfill the corresponding boundary conditions. These are given by

$$f(r_{c1}) = g(r_{c1}) \qquad g(r_{c2}) = 1 \tag{3.4}$$

$$f'(r_{c1}) = g'(r_{c1}) \qquad g'(r_{c2}) = 0 \tag{3.5}$$

$$f''(r_{c1}) = g''(r_{c1}) \qquad g''(r_{c2}) = 0 \tag{3.6}$$

The resulting system of linear equations for the coefficients $A - F$ is solved for the given values of r_{c1} and r_{c2}. Therefore, the complete Jastrow factor is given by

$$\tilde{f}_1(r) = \frac{1}{1 - \frac{a}{r_{c2}}} \cdot \begin{cases} 0 & \text{for } r \leq a \\ 1 - \frac{a}{r} & \text{for } a < r < r_{c1} \\ \sum_{i=0}^{5} a_i r^i & \text{for } r_{c1} < r < r_{c2} \end{cases} \tag{3.7}$$

Both versions of the first Jastrow factor f_1 are plotted in Fig. 3.1. It can be seen that the non-corrected factor according to Eq. 3.2 does not fulfill the requirements for periodic boundary conditions at $r_{c2} = L/2$.

As first step, an analytical expression for the local energy has to be found. Considering Eq. 2.6 leads to

$$\mathcal{H}\psi_T = -\sum_{k=1}^{N} \nabla_k^2 \psi_T = -\sum_{k=1}^{N} \nabla_k^2 \left[\prod_{i<j} \left(1 - \frac{a}{r_{ij}} \right) \right] \tag{3.8}$$

$$= -\sum_{k=1}^{N} \nabla_k^2 \left[\exp\left(\sum_{i<j} u(r_{ij}) \right) \right], \tag{3.9}$$

where $\hbar = 1$ and $m = 1/2$ is chosen and the function $u(r_{ij}) = \ln\left(1 - \frac{a}{r_{ij}}\right)$ has been

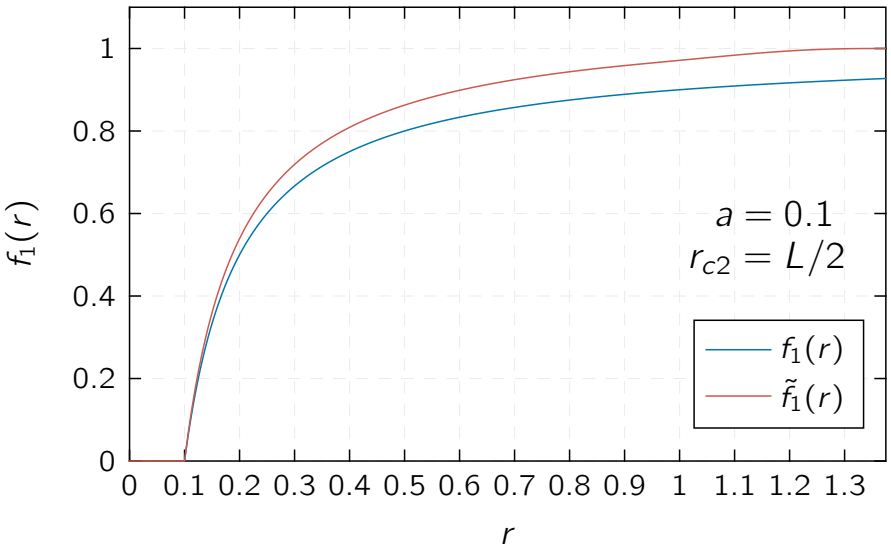

Figure 3.1: Jastrow factor plotted over absolute particle distance. Non-corrected $f_1(r)$ according to Eq. 3.2 (red) and the normalized Jastrow with smooth cutoff (blue).

introduced. The local energy can then be expressed as

$$E_l = \frac{\mathcal{H}\psi_T}{\psi_T} = -\sum_k \left[\left(\nabla_k \sum_{i<j} u(r_{ij}) \right)^2 + \nabla_k^2 \sum_{i<j} u(r_{ij}) \right] . \tag{3.10}$$

In particular, the local energy for the Jastrow factor given in Eq. 3.2 is calculated as

$$E_l^{(1)} = -\sum_{k=1}^{N} \left(\sum_{\substack{j=1 \\ j\neq k}}^{N} \frac{a}{1-\frac{a}{r_{kj}}} \frac{1}{r_{kj}^3} \boldsymbol{r}_{kj} \right)^2 + \sum_{\substack{j=1 \\ j\neq k}}^{N} \left(\frac{a^2}{\left(1-\frac{a}{r_{kj}}\right)^2} \frac{1}{r_{kj}^4} \right) \qquad \text{for } a < r < r_{c1} \tag{3.11}$$

$$E_{l,\text{cutoff}}^{(1)} = -\sum_{k=1}^{N} \left(\sum_{\substack{j=1 \\ j\neq k}}^{N} \frac{1}{\sum_{l=0}^{5} a_l r_{kj}^l} \sum_{l=1}^{5} l a_l r^{l-1} \frac{\boldsymbol{r}_{kj}}{r_{kj}} \right) + \sum_{\substack{j=1 \\ j\neq k}}^{N} \left[\frac{1}{\left(\sum_{l=0}^{5} a_l r_{kj}^l\right)^2} \left(\sum_{l=1}^{5} l a_l r_{kj}^{l-1} \right)^2 \right] \tag{3.12}$$

$$- \frac{1}{\sum_{l=0}^{5} a_l r_{kj}^l} \sum_{l=2}^{5} l(l-1) a_l r_{kj}^{l-2} \Bigg] \qquad \text{for } r_{c1} < r < r_{c2} \tag{3.13}$$

Now, the preparative calculations are completed and the Metropolis algorithm can be performed. The coordinate initialization places the particles on a lattice with lattice

constant $d = (1/\rho)^{1/3}$. Then, a particle is chosen randomly (uniform distribution) which is shifted in all three space dimensions by a random absolute value (Gaussian distribution).

```
unsigned n = dice_int(N-1);
for(unsigned j = 0; j < DIM; j++){
        coordinates[n][j] = GaussDistr(coordinates[n][j],cbrt(rho));
        coordinatesNIC[n][j] = get_coordinatesNIC(coordinates[n][j]);
}
```

Listing 2: Implementation of the random coordinate shift.

The particular implementation is shown in Listing 2. The argument of the function *GaussDistr* determines the mean (old coordinate) and the standard deviation ($\rho^{1/3}$) of the Gaussian distribution. After shifting the coordinates, the new positions are again back-projected regarding NIC.

With this new set of coordinates $\boldsymbol{R}'$ the wave function ratio $\left|\frac{\psi_T(\boldsymbol{R}')}{\psi_T(\boldsymbol{R})}\right|^2$ can be calculated. During the Metropolis algorithm, the new coordinates are accepted if $p < \left|\frac{\psi_T(\boldsymbol{R}')}{\psi_T(\boldsymbol{R})}\right|^2$, where p is a random real number between 0 and 1 (uniform distribution). Note that the overall acceptance ratio should be in the order of 50%.

For a chosen amount of 10^6 MC steps, every $m = 250$th step, the energy is updated. This yields a total summation of $P = 400$ calculated local energy terms given by Eq. 3.13 . The value of m should be chosen to be on the order of the particle number N, to ensure that every particle is moved once on average before calculating a new energy value. Therefore, the error bars can be calculated every time the energy is updated with

$$\sigma = \frac{1}{\sqrt{P}}\sqrt{\left|\frac{1}{P}\sum_p E_p^2 - \left(\frac{1}{P}\sum_p E_p\right)^2\right|} \,. \tag{3.14}$$

After exiting the Metropolis algorithm, the calculated ground state energy with error bars is given as output. For the weak scattering limit, i.e. $a\rho^{1/3} \ll 1$, the ground state energy per particle can be calculated analytically with the Gross-Pitaevskii (GP) equation and yields

$$\frac{E_0}{N} = a\rho\frac{4\pi\hbar^2}{m} \,. \tag{3.15}$$

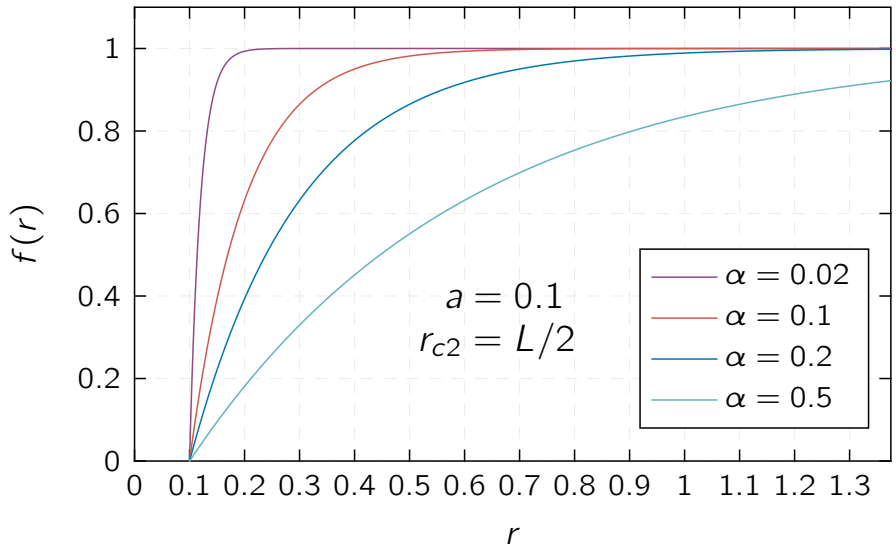

Figure 3.2: Jastrow factor according to Eq. 3.16 for different values of the optimization parameter α.

3.1.2 Trial wavefunction ansatz 2

The second Jastrow factor for the implementation in the VMC code is given by

$$f_2(r) = \begin{cases} 0 & \text{for } r \leq a \\ 1 - e^{-(r-a)/\alpha} & \text{for } r > a \end{cases} \tag{3.16}$$

The function defined as Jastrow factor in Eq. 3.16 is shown in Fig. 3.2 for different values of α.

Since the exponential function in Eq. 3.16 converges sufficiently fast to zero for small values of α, no smooth cutoff has to be applied to ensure periodic boundary conditions.

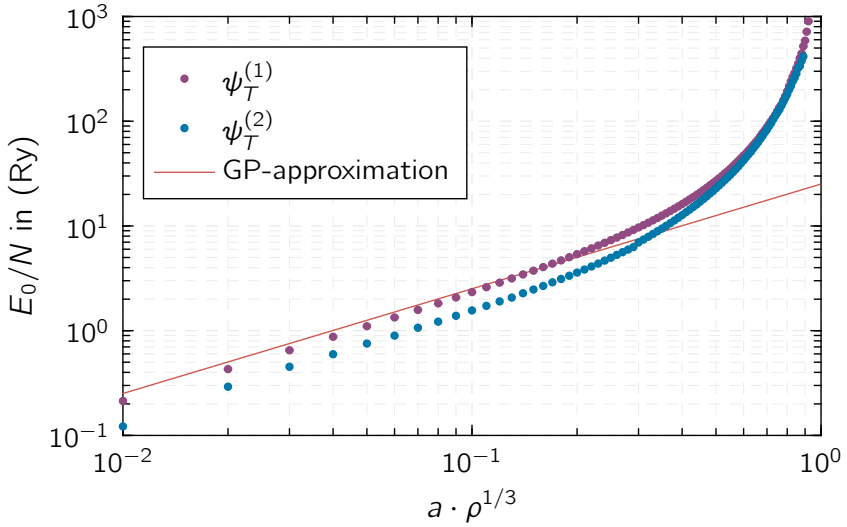

Figure 3.3: Total energy for both trial wavefunctions $\psi_T^{(1)}$ and $\psi_T^{(2)}$ for a system with $N = 343$ particles and $\rho = 1$. The parameter α for $\psi_T^{(2)}$ has been optimized for each value of $a\rho^{1/3}$.

The local energy calculated with Eq. 3.10 is expressed as

$$
\begin{aligned}
E_l^{(2)} = -\sum_{k=1}^{N} \Bigg[& \left(\frac{1}{\alpha} \sum_{\substack{j=1 \\ j\neq k}}^{N} \frac{\exp[-(r_{kj}-a)/\alpha]}{1-\exp[-(r_{kj}-a)/\alpha]} \frac{\boldsymbol{r}_{kj}}{r_{kj}} \right)^2 \\
& + \frac{1}{\alpha^2} \sum_{\substack{j=1 \\ j\neq k}}^{N} \left(\frac{\exp[-2(r_{kj}-a)/\alpha]}{(1-\exp[-(r_{kj}-a)/\alpha])^2} + \frac{\exp[-(r_{kj}-a)/\alpha]}{1-\exp[-(r_{kj}-a)/\alpha]} \right) \\
& - \frac{2}{\alpha} \sum_{\substack{j=1 \\ j\neq k}}^{N} \frac{\exp[-(r_{kj}-a)/\alpha]}{1-\exp[-(r_{kj}-a)/\alpha]} \frac{1}{r_{kj}} \Bigg]
\end{aligned}
$$

In contrast to the first Jastrow factor, the function according to Eq. 3.16 and the local energy $E_l^{(2)}$ contains now one optimization parameter α. For a fixed product $a\rho^{1/3}$ this parameter has been varied to find an optimal value that will minimize the energy of the system.

Varying both parameters (i.e. the system parameter $a\rho^{1/3}$ and the variational parameter α) gives a 3D map of the total energy showing the optimal variational parameter α for

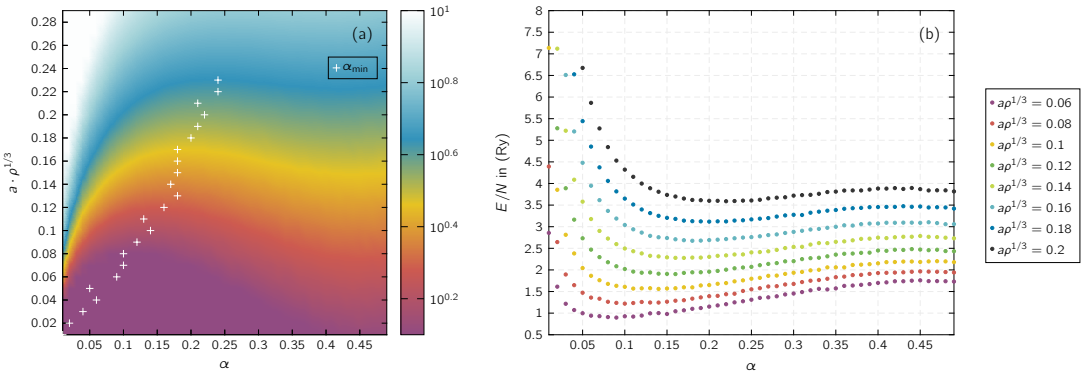

Figure 3.4: Total ground state energy in dependence of the variational parameter α and the product $a\rho^{1/3}$ for a simulation with $N = 343$ particles and $\rho = 1$. The white markers in (a) show the value of the variational parameter α that minimizes the ground state energy for a given value of $a\rho^{1/3}$.

every value of $a\rho^{1/3}$.

3.2 Results and discussion

For both trial wavefunctions, the ground state energy per particle E_0/N has been calculated and compared with the GP-approximation given by Eq. 3.15 . The number of particles is chosen to be $N = 343$ in all calculations. At the beginning of each simulation, the particle positions are initialized on a $7 \times 7 \times 7$ grid. It can be seen in Fig. 3.3 that in the low density limit, i.e. $a\rho^{1/3} \ll 1$ especially the first Jastrow factor, which does not contain any variational parameter, is in good agreement with the GP-approximation. The function given in Eq. 3.2 is actually the analytical result for the ground state energy if $N = 2$. In the dilute limit, this result seems to be a quite good approximation. For larger values of $a\rho^{1/3}$, the ground state energy calculated with the MC method increases drastically. In this case, strong correlations are expected and the GP-approximation does not hold. However, both Jastrow factors yield similar results. It has to be noted that for large values of $a\rho^{1/3}$ the second Jastrow factor would also need a cutoff correction in order to be able to reach lower ground state energies during the optimization process.
The optimization procedure of the second Jastrow factor is shown in Fig. 3.4(a). The ground state energy has been calculated for different values of the optimization parameter α and $a\rho^{1/3}$. In the dilute limit, very small values of α are preferred. For larger values of $a\rho^{1/3} \approx 0.1$ a minimum can be found at $\alpha \approx 0.13$ (cf. Fig. 3.4(b)). In order to better

identify the parameter value that corresponds to a minimum of the local energy it would be also possible to check for a variance minimum of the local energy, since this is also an indicator for the real ground state. However, for the present purpose, this procedure has not been performed.

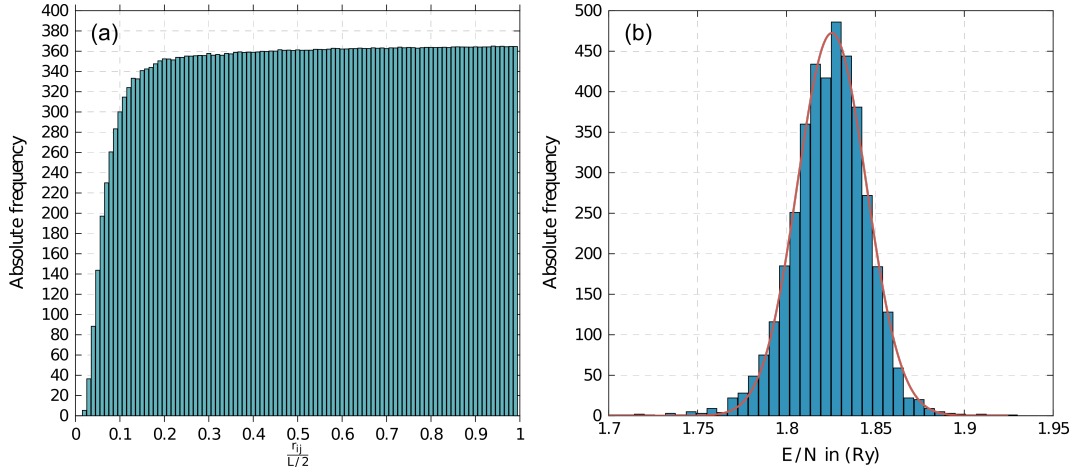

Figure 3.5: (a) Histogram of the interparticle distances inside the simulation cell up to a maximum distance of $L/2$ calculated for $N = 343$, $a = 0.08$ and $\rho = 1$. (b) Distribution of the individual energy summands in this simulation.

By considering the distribution of the particles within the box, the g_2-correlation function has been calculated in terms of a histogram. This behavior is shown in Fig. 3.5(a). At small particle distances the averaged probability distribution is nearly zero and increases with increasing distances. This is an indication for a correct movement of the particles, a smooth wave function ψ_T and a correct representation for periodic boundary conditions. When performing the MC integration for calculating the local energy E/N, the individual summands should be normally distributed around the expectation value of E/N. This can be seen in Fig. 3.5(b), where a Gaussian distribution function has been fitted to the histogram of energy values.

The energy values obtained with the VMC method are still approximations. The optimization parameter is actually chosen manually according to the variation principle by Ritz. A further improvement of QMC methods is the so-called *diffusion Monte Carlo* (DMC) method. Without going into detail, it has to be noted that the ground state energy obtained by DMC calculations is indeed exact within the fundamental statistical errors. It seems quite obvious that other expectation values than the ground state energy

can also be calculated with QMC methods. The DMC method yields only an exact value for the eigenvalue of the Hamilton operator. With even more sophisticated calculations, expectation values resulting from other operators may also be found exactly.

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