FYS4411 - Computational Physics II

Project 1

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February 14, 2018

Abstract

Write the abstract here

- Github repository containing programs and results are in: `https://github.com/evenmn/FYS4411/tree/master/Project%201`

1 Introduction

Introduction

2 Theory

We study a system of N bosons trapped in a harmonic oscillator with the Hamiltonian given by

$$\hat{H} = \sum_{i}^{N} \left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\vec{r}_i) \right) + \sum_{i<j}^{N} V_{int}(\vec{r}_i, \vec{r}_j) \tag{1}$$

with V_{ext} as the external potential, which is the harmonic oscillator potential, and V_{int} as the interaction term, which can be ignored when developing the benchmarks.

The wavefunction is on the form

$$\Psi_T(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, \alpha, \beta) = \prod_{i}^{N} g(\alpha, \beta, \vec{r}_i) \prod_{i<j} f(a, r_{ij}) \tag{2}$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ and g is assumed to be an exponential

$$g(\alpha, \beta, \vec{r}_i) = \exp[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)] \tag{3}$$

which is practical since

$$\prod_i^N g(\alpha, \beta, \vec{r}_i) = \exp[-\alpha(x_1^2 + y_1^2 + \beta z_1^2 + \cdots x_N^2 + y_N^2 + \beta z_N^2)]. \tag{4}$$

α is a variational parameter that we later use to find the energy minimum, and β is a constant. The f presented above is the correlation wave function, which is

$$f(a, r_{ij}) = \begin{cases} 0 & r_{ij} \leq a \\ \left(1 - \frac{a}{r_{ij}}\right) & r_{ij} > a. \end{cases} \tag{5}$$

The first case we will take into account, is when $a = 0$, and one might observe that $f = 1$ then. Anyway, ...

We want to calculate the local energy as a function of α, and then use Variational Monte Carlo (VMC) described in section 3.1. For the non-interacting case, the analytical expression is well-known and given by

$$E = \hbar\omega(n + 1/2) \tag{6}$$

where n is the total number of free dimensions, which gonna be an useful benchmark. The local energy is

$$E_L(\vec{r}) = \frac{1}{\Psi_T(\vec{r})} \hat{H} \Psi_T(\vec{r}) \tag{7}$$

which gives the following results considering $a = 0$:

INSERT ANALYTICAL EXPRESSIONS FROM A

For $a \neq 0$ it gets rather more complicated, because we need to deal with the correction wave function as well. By defining

$$f(a, r_{ij}) = \exp\left(\sum_{i<j} u(r_{ij})\right) \tag{8}$$

and doing a change of variables

$$\frac{\partial}{\partial r_k} = \frac{\partial}{\partial r_k}\frac{\partial r_{kj}}{\partial r_{kj}} = \frac{\partial r_{kj}}{\partial r_k}\frac{\partial}{\partial r_{kj}} = \frac{(r_k - r_j)}{r_{kj}}\frac{\partial}{\partial r_{kj}} \tag{9}$$

one will end up with

$$E_L = \sum_k \Bigg(-\frac{1}{2}\Bigg(4\alpha^2\Big(x_k^2 + y_k^2 + \beta^2 z_k^2 - \frac{1}{\alpha} - \frac{\beta}{2\alpha}\Big) \\ - 4\alpha \sum_{j\neq k} (x_k, y_k, \beta z_k) \frac{(\vec{r}_k - \vec{r}_j)}{r_{kj}} u'(r_{kj}) \\ + \sum_{ij\neq k} \frac{(\vec{r}_k - \vec{r}_j)(\vec{r}_k - \vec{r}_i)}{r_{ki} r_{kj}} u'(r_{ki}) u'(r_{kj}) \\ + \sum_{j\neq k} \Big(u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj}) \Big) \Bigg) + V_{ext}(\vec{r}_k) \Bigg). \tag{10}$$

This is not a pretty expression, but .. We could also split up the local energy expression

$$E_{L,i} = -\frac{\hbar^2}{2m} \frac{\nabla_i^2 \Psi_T}{\Psi_T} + V_{ext}(\vec{r}_i) = E_{k,i} + E_{p,i} \tag{11}$$

and calculate the local energy with a numerical approach where the second derivative can be approximated by the three-point formula:

$$f''(x) \simeq \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}. \tag{12}$$

In our case the position is a three dimensional vector, so we need to handle each dimension separately. However, in section 4.1, the CPU time for the analytical and numerical approach are compared.

3 Methods

3.1 Variational Monte Carlo

3.2 Metropolis algorithm

3.2.1 Brute force

3.2.2 Importance sampling

4 Results

4.1 CPU-time

For the brute force Metropolis algorithm we developed both an analytical and a numerical method to calculate the local energy. In table (1) we present the

results from these calculations and the performance. All the measurements are done in three dimensions with $\alpha = 0.5$ and $1e6$ Monte Carlo cycles. a is fixed to zero.

Table 1: Optimal parameters α and β and resulting energy E_{L2} and variance $\sigma_{E_{L2}}$ for different ω for Ψ_{T2}.

	Analytical		**Numerical**	
#Particles	$\langle E_L \rangle$ [..]	CPU-time [s]	$\langle E_L \rangle$ [..]	CPU-time [s]
1	1.50000	0.146392	1.49999	0.426018
10	15.000	11.8992	14.9999	38.0378
100				
500				

5 Discussion

6 Conclusion