Variational Monte Carlo on bosonic systems

Winther-Larsen, Sebastian Gregorius[1] and Schøyen, Øyvind Sigmundson[1]
[1] *University of Oslo*
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Something very abstract and clever should go here.

I. INTRODUCTION

We will in this project study the Variational Monte Carlo (VMC) method, and use it to evaluate the ground state energy of a trapped, hard sphere Bose gas.

II. THEORY

To model the trapped bosonic gas particles we use the potential

$$V_{\text{ext}}(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega^2 r^2 & \text{(S)}, \\ \frac{1}{2}m\left[\omega^2(x^2+y^2)+\omega_z^2 z^2\right] & \text{(E)}, \end{cases} \tag{1}$$

where we can choose between a spherical (S) or an elliptical (E) harmonic trap. The two-body Hamiltonian of the system is given by

$$H = \sum_i^N h(\mathbf{r}_i) + \sum_{i<j}^N w(\mathbf{r}_i, \mathbf{r}_j), \tag{2}$$

where the single particle one body operator, h, is given by

$$h(\mathbf{r}_i) = -\frac{\hbar^2}{2m}\nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i), \tag{3}$$

(we assume equal mass) and the two-body interaction operator, w, is

$$w(\mathbf{r}_i, \mathbf{r}_j) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a, \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a, \end{cases} \tag{4}$$

where a is the hard sphere of the particle. The trial wavefunction, $|\Psi_T\rangle$, we will be looking at is given by

$$\Psi_T(\mathbf{r}) = \Phi_T(\mathbf{r}) \prod_{j<k}^N f(a, \mathbf{r}_j, \mathbf{r}_k) \tag{5}$$

$$= \left(\prod_i^N g(\alpha, \beta, \mathbf{r}_i)\right) \prod_{j<k}^N f(a, \mathbf{r}_j, \mathbf{r}_k), \tag{6}$$

where α and β are variational parameters and

$$\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, \alpha, \beta). \tag{7}$$

Here g are the single particle wavefunctions given by

$$g(\alpha, \beta, \mathbf{r}_i) = \exp\left[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right] \equiv \phi(\mathbf{r}_i), \tag{8}$$

and $|\Phi_T\rangle$ the *Slater permanent* consisting of the N first single particle wavefunctions, and the correlation wavefunction, f, given by

$$f(a, \mathbf{r}_j, \mathbf{r}_k) = \begin{cases} 0 & |\mathbf{r}_j - \mathbf{r}_k| \leq a, \\ \left(1 - \frac{a}{|\mathbf{r}_j - \mathbf{r}_k|}\right) & |\mathbf{r}_j - \mathbf{r}_k| > a. \end{cases} \tag{9}$$

We will for brevity use the notation $\phi(\mathbf{r}_i) = \phi_i$ and $r_{jk} = |\mathbf{r}_j - \mathbf{r}_k|$.

A. Local energy

As the many-body wavefunction creates a very large configuration space, where much of the wavefunction is small, we use the Metropolis algorithm in order to move towards regions in configuration space with "sensible" values. We define the *local energy*, $E_L\mathbf{r}$, by

$$E_L(\mathbf{r}) = \frac{H\Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})}. \tag{10}$$

If $|\Psi_T\rangle$ is an exact eigenfunction of the Hamiltonian, E_L will be constant. The closer $|\Psi_T\rangle$ is to the exact wave function, the less variation in E_L as a function of $\mathbf{r}$ we get. One of the most computationally intensive parts of the VMC algorithm will be to compute E_L. We therefore find an analytical expression for E_L in terms of the trial wavefunction.

1. Non-interacting harmonic oscillator

We start by finding an analytical expression for the local energy in a system where we set $a = 0$ and $\beta = 1$, i.e., a system of non-interacting harmonic oscillators.

$$\Psi_T(\mathbf{r}) = \Phi_T(\mathbf{r}) = \prod_i^N \exp\left[-\alpha|\mathbf{r}_i|^2\right], \tag{11}$$

where $|\mathbf{r}_i| = r_i$. As $a = 0$ the interaction term, $w(\mathbf{r}_i, \mathbf{r}_j)$, vanishes and the Hamiltonian is given by (in the spherical case)

$$H = \sum_i^N h(\mathbf{r}_i) = \sum_i^N \left(-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}m\omega^2 r_i^2\right). \tag{12}$$

The hardest part of finding the local energy is computing the kinetic term. Starting with the gradient of the

wavefunction in the non-interacting case, we get

$$\nabla_k \Psi_T(\mathbf{r}) = -2\alpha \mathbf{r}_k \Psi_T(\mathbf{r}). \tag{13}$$

The Laplacian yields

$$\nabla_k^2 \Psi_T(\mathbf{r}) = \big(-2d\alpha + 4\alpha^2 r_k^2 \big) \Psi_T(\mathbf{r}), \tag{14}$$

where d is the dimensionality of the problem determined by $\mathbf{r}_k \in \mathbb{R}^d$. This yields the analytical expression for the local energy in the non-interacting case to be

$$E_L(\mathbf{r}) = \sum_i^N \left(-\frac{\hbar^2}{2m}\big[-2d\alpha + 4\alpha^2 r_i^2\big] + \frac{1}{2} m\omega^2 r_i^2 \right). \tag{15}$$

In natural units, with $\hbar = c = m = 1$, this reduces to

$$E_L(\mathbf{r}) = \alpha d N + \left(\frac{1}{2}\omega^2 - 2\alpha^2 \right) \sum_i^N r_i^2. \tag{16}$$

It is worth noting that for $\alpha = \frac{1}{2}\omega$ we will find a stable value. This happens as the entire sum over all the random walkers disappears.

2. The full system

Moving to the full system allowing β to vary and setting $a \neq 0$ we write the trial wavefunction as

$$\Psi_T(\mathbf{r}) = \Phi_T(\mathbf{r}) J(\mathbf{r}), \tag{17}$$

where $|\Phi_T\rangle$ is the same Slater permanent as in Equation 6 and $J(\mathbf{r})$ is the *Jastrow factor* given by

$$J(\mathbf{r}) = \exp\left(\sum_{j<l}^N u(r_{jl}) \right), \tag{18}$$

where $r_{jk} = |\mathbf{r}_j - \mathbf{r}_k|$ and

$$u(r_{jk}) = \ln\big[f(a, \mathbf{r}_j, \mathbf{r}_k) \big]. \tag{19}$$

To further shorten the notation we will use $u_{jk} = u(r_{jk})$. We wish to find an analytical expression for the local energy. Beginning with the gradient we get

$$\nabla_k \Psi_T(\mathbf{r}) = \Big[\nabla_k \Phi_T(\mathbf{r}) \Big] J(\mathbf{r}) + \Phi_T(\mathbf{r}) \nabla_k J(\mathbf{r}). \tag{20}$$

The gradient of the Slater permament for particle k is given by

$$\nabla_k \Phi_T(\mathbf{r}) = \nabla_k \phi_k \prod_{i \neq k}^N \phi_i = \frac{\nabla_k \phi_k}{\phi_k} \Phi_T(\mathbf{r}). \tag{21}$$

The gradient of the Jastrow factor is given by

$$\nabla_k J(\mathbf{r}) = J(\mathbf{r}) \nabla_k \sum_{m<n}^N u_{mn} \tag{22}$$

$$= J(\mathbf{r}) \left(\sum_{m=1}^{k-1} \nabla_k u_{mk} \sum_{n=k+1}^N \nabla_k u_{kn} \right) \tag{23}$$

$$= J(\mathbf{r}) \sum_{m \neq k}^N \nabla_k u_{km}, \tag{24}$$

where the gradient of the interaction term splits the anti-symmetric sum into two parts. As $r_{ij} = r_{ji}$ we can combine these sums into a single sum. This in total yields the gradient

$$\nabla_k \Psi_T(\mathbf{r}) = \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{m \neq k}^N \nabla_k u_{km} \right) \Psi_T(\mathbf{r}). \tag{25}$$

We now find the Laplacian of the trial wavefunction by finding the divergence of Equation 25.

$$\nabla_k^2 \Psi_T(\mathbf{r}) = \left(\nabla_k \left[\frac{\nabla_k \phi_k}{\phi_k} \right] + \sum_{m \neq k}^N \nabla_k^2 u_{km} \right) \Psi_T(\mathbf{r}) \tag{26}$$

$$+ \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{m \neq k}^N \nabla_k u_{km} \right)^2 \Psi_T(\mathbf{r}), \tag{27}$$

where the squared term came from taking the gradient of the trial wavefunction. To further simplify we divide by the trial wavefunction. This yields

$$\frac{\nabla_k^2 \Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = \left(\nabla_k \left[\frac{\nabla_k \phi_k}{\phi_k} \right] + \sum_{m \neq k}^N \nabla_k^2 u_{km} \right) + \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{m \neq k}^N \nabla_k u_{km} \right)^2 \tag{28}$$

$$= \frac{\nabla_k^2 \phi_k}{\phi_k} + 2 \frac{\nabla_k \phi_k}{\phi_k} \sum_{m \neq k}^N \nabla_k u_{km} + \sum_{m \neq k}^N \nabla_k^2 u_{km} + \left(\sum_{m \neq k}^N \nabla_k u_{km} \right)^2. \tag{29}$$

To go from here we have to find the gradient and the Laplacian of the single particle functions, ϕ_k, and the interaction functions u_{km}. For the single particle functions we use Cartesian coordinates when finding the derivatives whereas we for the interaction functions will use spherical coordinates and do a variable substitution. Beginning with the gradient of the single particle functions we get

$$\nabla_k \phi_k = \nabla_k \exp\left[-\alpha(x_k^2 + y_k^2 + \beta z_k^2)\right] \tag{30}$$
$$= -2\alpha(x_k \mathbf{e}_i + y_k \mathbf{e}_j + \beta z_k \mathbf{e}_k)\phi_k. \tag{31}$$

Note that the subscripts on the unit vectors $\mathbf{e}_i$ are *not* the same as the subscripts used for its components. The Laplacian yields

$$\nabla_k^2 \phi_k = \Big[-2\alpha\big(2+\beta\big) + 4\alpha^2\big(x_k^2 + y_k^2 + \beta^2 z_k^2\big)\Big]\phi_k. \tag{32}$$

In order to derive the interaction functions we have to do a variable substitution using $r_{km} = |\mathbf{r}_k - \mathbf{r}_m|$. We can then rewrite the ∇_k-operator as

$$\nabla_k = \nabla_k \frac{\partial r_{km}}{\partial r_{km}} = \nabla_k r_{km} \frac{\partial}{\partial r_{km}} \tag{33}$$
$$= \frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}} \frac{\partial}{\partial r_{km}}. \tag{34}$$

Applying this version of the ∇_k-operator to u_{km} yields

$$\nabla_k u_{km} = \frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}} \frac{\partial u_{km}}{\partial r_{km}}. \tag{35}$$

For the Laplacian we switch a little back and forth between the two ways of representing the ∇_k-operator. We thus get

$$\nabla_k^2 u_{km} = \frac{\nabla_k \mathbf{r}_k}{r_{km}} \frac{\partial u_{km}}{\partial r_{km}} + \left[\nabla_k \frac{1}{r_{km}}\right](\mathbf{r}_k - \mathbf{r}_m) \frac{\partial u_{km}}{\partial r_{km}} + \frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}} \nabla_k \frac{\partial u_{km}}{\partial r_{km}} \tag{36}$$
$$= \frac{d}{r_{km}} \frac{\partial u_{km}}{\partial r_{km}} - \frac{(\mathbf{r}_k - \mathbf{r}_m)^2}{r_{km}^3} \frac{\partial u_{km}}{\partial r_{km}} + \frac{(\mathbf{r}_k - \mathbf{r}_m)^2}{r_{km}^2} \frac{\partial^2 u_{km}}{\partial r_{km}^2} \tag{37}$$
$$= \frac{d-1}{r_{km}} \frac{\partial u_{km}}{\partial r_{km}} + \frac{\partial^2 u_{km}}{\partial r_{km}^2}, \tag{38}$$

where d is again the dimensionality of the problem. In total we can state an intermediate version of the Laplacian occuring in the local energy as

$$\frac{\nabla_k^2 \Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = \frac{\nabla_k^2 \phi_k}{\phi_k} + 2\frac{\nabla_k \phi_k}{\phi_k} \sum_{m \neq k}^{N} \frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}} \frac{\partial u_{km}}{\partial r_{km}} + \sum_{m \neq k}^{N} \left(\frac{d-1}{r_{km}} \frac{\partial u_{km}}{\partial r_{km}} + \frac{\partial^2 u_{km}}{\partial r_{km}^2} \right)$$
$$+ \sum_{m,n \neq k}^{N} \frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}} \frac{\mathbf{r}_k - \mathbf{r}_n}{r_{kn}} \frac{\partial u_{km}}{\partial r_{km}} \frac{\partial u_{kn}}{\partial r_{kn}}. \tag{39}$$

Moving on to the derivatives of the interaction terms, u_{km}, to get an explicit expression for the Laplacian.

$$\frac{\partial u_{km}}{\partial r_{km}} = \frac{a}{r_{km}(r_{km} - a)}, \tag{40}$$
$$\frac{\partial^2 u_{km}}{\partial r_{km}^2} = \frac{a^2 - 2a r_{km}}{r_{km}^2 (r_{km} - a)^2}. \tag{41}$$