Variational Monte Carlo on bosonic systems

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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

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

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 we will be looking at is given by

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

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

where α and β are variational parameters and

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

Here g are the single particle wavefunctions given by

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

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

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

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

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

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 part 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 with a system where we set $a = 0$ and $\beta = 1$, i.e., a system of non-interacting harmonic oscillators.

$$\langle \mathbf{r}|\Psi_T\rangle = \langle \mathbf{r}|\Phi_T\rangle = \prod_i^N \exp\big[-\alpha|\mathbf{r}_i|^2\big], \tag{11}$$

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)

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

Working in spherical coordinates the gradient and the Laplace operator (applied to a scalar function) becomes

$$\nabla f = \mathbf{e}_r \partial_r f + \mathbf{e}_\theta \frac{1}{r}\partial_\theta f + \mathbf{e}_\phi \frac{1}{r\sin(\theta)}\partial_\phi f, \tag{13}$$

$$\nabla^2 f = \frac{1}{r^2}\partial_r\left[r^2\partial_r f\right] + \frac{1}{r^2\sin(\theta)}\partial_\theta\left[\sin(\theta)\partial_\theta f\right] + \frac{1}{r^2\sin^2(\theta)}{\partial_\phi}^2 f, \tag{14}$$

where $\mathbf{e}_r$ signifies the unit vector in the radial direction and we use the shorthand notation

$$\partial_r f \equiv \frac{\partial f}{\partial r}. \tag{15}$$

As the trial wavefunction for $\beta = 1$ is purely radial we get the same expression in one, two and three dimensions by setting

$$r^2 = \begin{cases} x^2 & \text{one dimension,} \\ x^2 + y^2 & \text{two dimensions,} \\ x^2 + y^2 + z^2 & \text{three dimensions.} \end{cases} \tag{16}$$

The gradient then becomes

$$\nabla_i \langle \mathbf{r}|\Psi_T\rangle = \mathbf{e}_{r_i}\partial_{r_i}\prod_j^N \exp\left[-\alpha r_j^2\right] \tag{17}$$

$$= -2\alpha r_i \prod_j^N \exp\left[-\alpha r_j^2\right]\mathbf{e}_{r_i} \tag{18}$$

$$= -2\alpha r_i \langle \mathbf{r}|\Psi_T\rangle \mathbf{e}_{r_i}. \tag{19}$$

The Laplacian is given by

$$\nabla_i^2 \langle \mathbf{r}|\Psi_T\rangle = \frac{1}{r_i^2}\partial_{r_i}\left\{r_i^2\partial_{r_i}\prod_j^N \exp\left[-\alpha r_j^2\right]\right\} \tag{20}$$

$$= \frac{1}{r_i^2}\partial_{r_i}\left\{-2\alpha r_i^3\prod_j^N \exp\left[-\alpha r_j^2\right]\right\} \tag{21}$$

$$= \frac{1}{r_i^2}\left\{-6\alpha r_i^2 + 4\alpha^2 r_i^4\right\}\prod_j^N \exp\left[-\alpha r_j^2\right] \tag{22}$$

$$= \left\{-6\alpha + 4\alpha^2 r_i^2\right\}\langle \mathbf{r}|\Psi_T\rangle. \tag{23}$$

This gives the analytical expression for the local energy to be

$$E_L(\mathbf{r}) = \frac{\langle \mathbf{r}| H |\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} \tag{24}$$

$$= \sum_i^N\left(4\alpha^2 r_i^2 + \frac{1}{2}m\omega^2 r_i^2\right) - 6\alpha. \tag{25}$$

The *drift force* of the system is given by

$$\mathbf{F}_i = \frac{2\nabla_i \langle \mathbf{r}|\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} \tag{26}$$

$$= -4\alpha r_i \mathbf{e}_{r_i}. \tag{27}$$

2. The full system

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

$$\langle \mathbf{r}|\Psi_T\rangle = \langle \mathbf{r}|\Phi_T\rangle J(\mathbf{r}), \tag{28}$$

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

$$J(\mathbf{r}) = \exp\left(\sum_{j<l}^N u(r_{jl})\right), \tag{29}$$

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

$$u(r_{jk}) = \ln\left[f(a, \mathbf{r}_j, \mathbf{r}_k)\right]. \tag{30}$$

We wish to find an analytical expression for the local energy. Beginning with the gradient we get

$$\nabla_k \langle \mathbf{r}|\Psi_T\rangle = \nabla_k\Big[\langle \mathbf{r}|\Phi_T\rangle J(\mathbf{r})\Big] \tag{31}$$

$$= \Big[\nabla_k \langle \mathbf{r}|\Phi_T\rangle\Big] J(\mathbf{r}) + \langle \mathbf{r}|\Phi_T\rangle \nabla_k J(\mathbf{r}). \tag{32}$$

The gradient of the Slater permanent gives

$$\nabla_k \langle \mathbf{r}|\Phi_T\rangle = \nabla_k\phi(\mathbf{r}_k)\prod_{i\neq k}^N \phi(\mathbf{r}_i) \tag{33}$$

$$= \frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\langle \mathbf{r}|\Phi_T\rangle. \tag{34}$$

The gradient of the Jastrow factor is given by

$$\nabla_k J(\mathbf{r}) = J(\mathbf{r})\nabla_k \sum_{m<n}^{N} u(r_{mn}) \tag{35}$$

$$= J(\mathbf{r})\left(\sum_{m=1}^{k-1} \nabla_k u(r_{mk}) + \sum_{n=k+1}^{N} \nabla_k u(r_{kn})\right) \tag{36}$$

$$= J(\mathbf{r}) \sum_{m\neq k}^{N} \nabla_k u(r_{km}), \tag{37}$$

as $r_{ij} = r_{ji}$. We are thus left with

$$\nabla_k \langle \mathbf{r}|\Psi_T\rangle = \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \langle \mathbf{r}|\Psi_T\rangle + \langle \mathbf{r}|\Psi_T\rangle \sum_{m\neq k}^{N} \nabla_k u(r_{km}) \tag{38}$$

$$= \left(\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{m\neq k}^{N} \nabla_k u(r_{km})\right) \langle \mathbf{r}|\Psi_T\rangle . \tag{39}$$

We can now find the Laplacian of the trial wavefunction. This gives

$$\nabla_k^2 \langle \mathbf{r}|\Psi_T\rangle = \nabla_k \nabla_k \langle \mathbf{r}|\Psi_T\rangle = \nabla_k \left(\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{m\neq k}^{N} \nabla_k u(r_{km})\right) \langle \mathbf{r}|\Psi_T\rangle \tag{40}$$

$$= \left(\frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \left[\nabla \frac{1}{\phi(\mathbf{r}_k)}\right] \nabla_k \phi(\mathbf{r}_k) + \sum_{m\neq k}^{N} \nabla_k^2 u(r_{km})\right) \langle \mathbf{r}|\Psi_T\rangle \tag{41}$$

$$+ \left(\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{m\neq k}^{N} \nabla_k u(r_{km})\right) \nabla_k \langle \mathbf{r}|\Psi_T\rangle \tag{42}$$

$$= \left(\frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} - \left[\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\right]^2 + \sum_{m\neq k}^{N} \nabla_k^2 u(r_{km})\right) \langle \mathbf{r}|\Psi_T\rangle \tag{43}$$

$$+ \left(\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{m\neq k}^{N} \nabla_k u(r_{km})\right)^2 \langle \mathbf{r}|\Psi_T\rangle . \tag{44}$$

We now divide by the trial wavefunction. This simplifies the calculations and is more similar to the expression for the local energy.

$$\frac{\nabla_k^2 \langle \mathbf{r}|\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} = \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} - \left[\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\right]^2 + \sum_{m\neq k}^{N} \nabla_k^2 u(r_{km}) + \left(\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{m\neq k}^{N} \nabla_k u(r_{km})\right)^2 \tag{45}$$

$$= \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{m\neq k}^{N} \nabla_k^2 u(r_{km}) + \frac{2\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{m\neq k}^{N} \nabla_k u(r_{km}) + \left(\sum_{m\neq k}^{N} \nabla_k u(r_{km})\right)^2 \tag{46}$$

To go from here we have to find the gradient and the Laplacian of the single particle functions, $\phi(\mathbf{r}_k)$, and the interaction functions $u(r_{km})$. 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

$$\nabla_k \phi(\mathbf{r}_k) = \nabla_k \exp\left[-\alpha(x_k^2 + y_k^2 + \beta z_k^2)\right] \tag{47}$$

$$= -2\alpha(x_k \mathbf{e}_i + y_k \mathbf{e}_j + \beta z_k \mathbf{e}_k)\phi(\mathbf{r}_k), \tag{48}$$

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

$$\nabla_k^2\phi(\mathbf{r}_k) = -2\alpha\big(2+\beta\big)\phi(\mathbf{r}_k) + 4\alpha^2\big(x_k^2+y_k^2+\beta^2 z_k^2\big)\phi(\mathbf{r}_k). \tag{49}$$

In order to derive the interaction functions we have to do a variable substitution. We replace the derivative of the radial component for particle k by

$$\partial_{r_k} = \frac{\partial r_{km}}{\partial r_k}\,\partial_{r_{km}}. \tag{50}$$

The derivative of the distance r_{km} is given by

$$r_{km} = |\mathbf{r}_k - \mathbf{r}_m| \implies \frac{\partial r_{km}}{\partial r_k} = \frac{r_k - r_m}{|\mathbf{r}_k - \mathbf{r}_m|}, \tag{51}$$

where in spherical coordinates $\mathbf{r}_k = r_k\mathbf{e}_r$. The gradient of $u(r_{km})$ thus simplifies to only include the radial contribution.

$$\begin{aligned}
\nabla_k u(r_{km}) &= \mathbf{e}_r\partial_{r_k} u(r_{km}) && (52)\\
&= \mathbf{e}_r\,\frac{\partial r_{km}}{\partial r_k}\,\partial_{r_{km}} u(r_{km}) && (53)\\
&= \mathbf{e}_r\frac{r_k - r_m}{r_{km}}\partial_{r_{km}} u(r_{km}). && (54)
\end{aligned}$$

Using this expression we find the Laplacian to be

$$\begin{aligned}
\nabla_k^2 u(r_{km}) &= \frac{1}{r_{km}}\partial_{r_{km}} u(r_{km}) + \frac{(r_k - r_m)^2}{r_{km}^3}\partial_{r_{km}} u(r_{km}) + \frac{r_k - r_m}{r_{km}}\,\frac{\partial r_{km}}{\partial r_k}\,\partial_{r_{km}}^2 u(r_{km}) && (55)\\
&= \frac{1}{r_{km}}\partial_{r_{km}} u(r_{km}) + \frac{r_{km}^2}{r_{km}^3}\partial_{r_{km}} u(r_{km}) + \frac{(r_k - r_m)^2}{r_{km}^2}\partial_{r_{km}}^2 u(r_{km}) && (56)\\
&= \frac{2}{r_{km}}\partial_{r_{km}} u(r_{km}) + \partial_{r_{km}}^2 u(r_{km}). && (57)
\end{aligned}$$

We now take the derivate with respect to r_{km} of the interaction functions $u(r_{km})$ to find the closed form expressions. We get

$$\begin{aligned}
\partial_{r_{km}} u(r_{km}) &= \partial_{r_{km}} \ln\left(1 - \frac{a}{r_{km}}\right) && (58)\\
&= \partial_{r_{km}} \ln\left(\frac{1}{r_{km}}(r_{km} - a)\right) && (59)\\
&= \partial_{r_{km}}\Big[\ln(r_{km} - a) - \ln(r_{km})\Big] && (60)\\
&= \frac{1}{r_{km} - a} - \frac{1}{r_{km}} && (61)\\
&= \frac{a}{r_{km}(r_{km} - a)} && (62)\\
\partial_{r_{km}}^2 u(r_{km}) &= a\Big(\partial_{r_{km}}\frac{1}{r_{km}}\Big)\partial_{r_{km}}\frac{1}{r_{km} - a} \\
&\quad + a\frac{1}{r_{km}}\Big(\partial_{r_{km}}\frac{1}{r_{km} - a}\Big) && (63)\\
&= -\frac{a}{r_{km}^2(r_{km} - a)} - \frac{a}{r_{km}(r_{km} - a)^2} && (64)\\
&= -\frac{2a(r_{km} - 1)}{r_{km}^2(r_{km} - a)^2}. && (65)
\end{aligned}$$

Using this we are now able to write the closed form expression of the Laplacian of the trial wavefunction.

$$\frac{\nabla_k^2 \langle \mathbf{r}|\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} = -2\alpha\big(2+\beta\big) + 4\alpha^2\big(x_k^2 + y_k^2 + \beta^2 z_k^2\big) + 2a\sum_{m\neq k}^{N}\left[\frac{1}{r_{km}^2(r_{km}-a)} - \frac{r_{km}-1}{r_{km}^2(r_{km}-a)^2}\right]$$
$$- 4\alpha(x_k\mathbf{e}_i + y_k\mathbf{e}_j + \beta z_k\mathbf{e}_k)\cdot a\sum_{m\neq k}^{N}\frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}^2(r_{km}-a)} + \left[a\sum_{m\neq k}^{N}\frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}^2(r_{km}-a)}\right]^2. \tag{66}$$

To ease the load on the CPU we try to restrict the number of times we evaluate the sums. For brevity we introduce the following functions

$$\xi_k(\mathbf{r}, a) = \sum_{m\neq k}^{N}\left[\frac{1}{r_{km}^2(r_{km}-a)} - \frac{r_{km}-1}{r_{km}^2(r_{km}-a)^2}\right] \tag{67}$$

$$= \sum_{m\neq k}^{N}\frac{1-a}{r_{km}^2(r_{km}-a)^2}, \tag{68}$$

$$\boldsymbol{\zeta}_k(\mathbf{r}, a) = \sum_{m\neq k}^{N}\frac{\mathbf{r}_k - \mathbf{r}_m}{r_{km}^2(r_{km}-a)}. \tag{69}$$

We can then rewrite the expression for the Laplacian to

$$\frac{\nabla_k^2 \langle \mathbf{r}|\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} = -2\alpha\big(2+\beta\big) + 4\alpha^2\big(x_k^2 + y_k^2 + \beta^2 z_k^2\big) + 2a\xi_k(\mathbf{r}, a)$$
$$- 4a\alpha(x_k\mathbf{e}_i + y_k\mathbf{e}_j + \beta z_k\mathbf{e}_k)\cdot\boldsymbol{\zeta}_k(\mathbf{r}, a) + a^2\boldsymbol{\zeta}_k(\mathbf{r}, a)^2. \tag{70}$$

Both ξ_k and $\boldsymbol{\zeta}_k$ can be evaluated in a common loop. Using this expression for the Laplacian we can find the local energy from

$$E_L(\mathbf{r}) = \frac{\langle \mathbf{r}|\, H\, |\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} = \sum_{k}^{N}\left(-\frac{\hbar^2}{2m}\frac{\nabla_k^2 \langle \mathbf{r}|\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle} + V_{\text{ext}}(\mathbf{r})\right) + \sum_{i<j}^{N} w(\mathbf{r}_i, \mathbf{r}_j). \tag{71}$$