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

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

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 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

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

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

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

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.

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

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)

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

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

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

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

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

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

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

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

The Laplacian is given by

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

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

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

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

This gives the analytical expression for the local energy to be

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

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

The *drift force* of the system is given by

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

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

2. The full system

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

$$\langle \mathbf{r} | \Psi_T \rangle = \langle \mathbf{r} | \Phi_T \rangle \exp\left(\sum_{j<k}^N u(r_{jk}) \right) \tag{28}$$

$$= \left(\prod_i^N \phi(\mathbf{r}_i) \right) \exp\left(\sum_{j<k}^N u(r_{jk}) \right), \tag{29}$$

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

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

we wish to compute the local energy. The gradient is thus given by

$$\langle \mathbf{r}| \nabla_k |\Psi_T\rangle = \nabla_k \left\{ \langle \mathbf{r}|\Phi_T\rangle \exp\left(\sum_{j<l}^{N} u(r_{jl})\right)\right\} \tag{31}$$

$$= \left\{\nabla_k \prod_i^N \phi(\mathbf{r}_i)\right\} \exp\left(\sum_{j<l}^{N} u(r_{jl})\right) + \langle \mathbf{r}|\Phi_T\rangle \nabla_k \exp\left(\sum_{j<l}^{N} u(r_{jl})\right) \tag{32}$$

$$= \left\{\nabla_k \phi(\mathbf{r}_k) \prod_{i\neq k}^N \phi(\mathbf{r}_i)\right\} \exp\left(\sum_{j<l}^{N} u(r_{jl})\right) + \langle \mathbf{r}|\Psi_T\rangle \nabla_k \left(\sum_{m<n}^{N} u(r_{mn})\right). \tag{33}$$

The last term is extracted from the chain rule and can be evaluated as

$$\nabla_k \sum_{m<n}^{N} u(r_{mn}) = \sum_{m=1}^{k-1} \nabla_k u(r_{mk}) + \sum_{n=k+1}^{N} \nabla_k u(r_{kn}) \tag{34}$$

$$= \sum_{m\neq k}^{N} \nabla_k u(r_{km}), \tag{35}$$

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

$$\langle \mathbf{r}| \nabla_k |\Psi_T\rangle = \left\{\nabla_k \phi(\mathbf{r}_k) \prod_{i\neq k}^N \phi(\mathbf{r}_i)\right\} \exp\left(\sum_{j<k}^{N} u(r_{jk})\right) + \langle \mathbf{r}|\Psi_T\rangle \sum_{m\neq k}^{N} \nabla_k u(r_{km}). \tag{36}$$