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

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

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

$$\Psi_T(\mathbf{r}) = \langle \mathbf{r}|\Psi_T\rangle = \prod_i^N g(\alpha,\beta,\mathbf{r}_i)\prod_{i<j}^N f(a,\mathbf{r}_i,\mathbf{r}_j), \tag{5}$$

where α and β are variational parameters and

$$\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, \alpha, \beta). \tag{6}$$

Here g are the single-particle wavefunctions given by

$$g(\alpha,\beta,\mathbf{r}_i) = \exp\left[-\alpha(x_i^2+y_i^2+\beta z_i^2)\right] \equiv \phi(\mathbf{r}_i), \tag{7}$$

and the correlation wavefunction, f, is

$$f(a,\mathbf{r}_i,\mathbf{r}_j) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a, \\ \left(1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}\right) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \tag{8}$$

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

$$E_L(\mathbf{r}) = \frac{\langle \mathbf{r}|\, H\, |\Psi_T\rangle}{\langle \mathbf{r}|\Psi_T\rangle}. \tag{9}$$

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 $a = 0$ and $\beta = 1$, i.e., a non-interaction harmonic oscillator given by the wavefunction

$$\langle \mathbf{r}|\Psi_T\rangle = \prod_i^N \exp\left[-\alpha|\mathbf{r}_i|^2\right], \tag{10}$$

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)

$$H = \sum_i^N h(\mathbf{r}_i) = \sum_i^N \Big(-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}m\omega^2 r_i^2.\Big) \tag{11}$$