# 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

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

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

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

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

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

and the two-body interaction operator, $w$, is

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

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

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

where $\alpha$ and $\beta$ are variational parameters and

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

Here $g$ are the single-particle wavefunctions given by

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

and the correlation wavefunction, $f$, is

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