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

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

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.