FYS4411 - Computational quantum mechanics

Spring 2016

Project 1; Variational Monte Carlo Studies of Bosonic systems

temporary report

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Date: February 6, 2016

Abstract

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2.1.1 Simplified problem

The local energy is defined as:

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} H\Psi_T(\mathbf{R}), \tag{1}$$

As a first approximation, it is assumed there is no interaction term in the Hamiltonian, which means the hard sphere bosons have no physical size (the hard-core diameter is zero). It is also assumed that no magnetic field is applied to the bosonic gas, leaving a perfectly spherically symmetrical harmonic trap. Inserting this new Hamiltonian into the local energy gives:

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} \sum_i^N \left(\frac{-\hbar^2}{2m}\nabla_i^2 + \frac{1}{2} m\omega_{ho}^2 r_i^2 \right) \Psi_T(\mathbf{R}) \tag{2}$$

The potential term is trivial since this is a scalar, i.e. the denominator will cancel the wavefunction. A more challenging problem is to find an expression for $\nabla_i^2 \Psi_T(\mathbf{R})$. The trial wavefunction shown in equation (...), with the aforementioned approximations, is:

$$\Psi_T(\mathbf{R}) = \prod_i e^{-\alpha r_i^2} \tag{3}$$

where α is the variational parameter for VCM. The first derivative is:

$$\nabla_j \prod_i e^{-\alpha r_i^2} = -2\alpha \mathbf{r}_j e^{-\alpha r_j^2} \prod_{i \neq j} e^{-\alpha r_i^2} \tag{4}$$

$$= -2\alpha \mathbf{r}_j \prod_i e^{-\alpha r_i^2}. \tag{5}$$

The second derivative then follows:

$$\nabla_j^2 \prod_i e^{-\alpha r_i^2} = \nabla_j \left(-2\alpha \mathbf{r}_j \prod_i e^{-\alpha r_i^2} \right) \tag{6}$$

$$= \left(4\alpha^2 r_j^2 - 2d\alpha\right) \prod_i e^{-\alpha r_i^2}. \tag{7}$$

where d is the number of dimensions. Inserting this into back into the local energy (equation (2)), the final expression can be derived:

$$\begin{aligned} E_L(\mathbf{R}) &= \frac{1}{\Psi_T(\mathbf{R})} \sum_i^N \left(\frac{-\hbar^2}{2m}\nabla_i^2 + \frac{1}{2} m\omega_{ho}^2 r^2 \right) \Psi_T(\mathbf{R}) \\ &= \sum_{i=1}^N \left[\frac{-\hbar^2}{2m} \left(4\alpha^2 r_i^2 - 2d\alpha\right) + \frac{1}{2} m\omega_{ho}^2 r_i^2 \right] \end{aligned}$$

The drift force (quantum force), still with the approximations above, is defined by:

$$F = \frac{2\nabla\Psi_T}{\Psi_T} \tag{8}$$

The gradient here is defined as

$$\nabla \equiv (\nabla_1, \nabla_2, \ldots, \nabla_N)$$

i.e. a vector of dimension Nd. The gradient with respect to a single particle's position is already given in equation 5, so it's not too hard to see the following is the necessary factor in the drift force:

$$F = \frac{-4\alpha}{\Psi_T}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right)\Psi_T$$
$$= -4\alpha\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right)$$

2.1.2 Full problem

The full problem[1] is a bit more tedious to derive. The first step is to rewrite the trial wavefunction to the following form:

$$\Psi_T(\mathbf{R}) = \prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \tag{9}$$

where, in order for this to fit with the previous wavefunction, $u(r_{ij}) \equiv \ln(f(r_{ij}))$ and $\phi(\mathbf{r}_i) \equiv g(\alpha, \beta, \mathbf{r}_i)$. The gradient with respect to the k-th coordinate set is:

$$\nabla_k \Psi_T = \nabla_k \prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \tag{10}$$
$$= \nabla_k \phi_k \left[\prod_{i \neq k} \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})}\right] + \left[\prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \nabla_k \left(\sum_{i''<j''} u_{i''j''}\right)\right] \tag{11}$$
$$= \nabla_k \phi_k \left[\prod_{i \neq k} \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})}\right] + \left[\prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \left(\sum_{i''<j''} \nabla_k u_{i''j''}\right)\right] \tag{12}$$

The function u_{ij} is symmetric under permutation of i and j, as one can see from the definitions of itself and $f(r_{ij})$. This means that in the last sum above, one can always s

3 Results

4 Conclusions

5 Appendix

[1]The "full problem" means not making any assumptions on the particle interactions or the potential.