FYS4411 - Project 1
Variational Monte Carlo

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Abstract

Abstract awesomeness

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A Finding the analytic expression for the local energy

We wish to find:

$$E_L = \frac{1}{\Psi_T}\nabla^2\Psi_T \tag{1}$$

Where Ψ_T is given by:

$$\exp\left[-\alpha\sum_i^n\left(x_i^2+y_i^2+z_i^2\right)\right]\prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) \tag{2}$$

Look first at $a = 0$. In this case, this reduces to the harmonic oscillator potential. The local energy is then:

$$\exp\left[\alpha \sum_{i}^{n} \left(x_i^2 + y_i^2 + z_i^2\right)\right] \left(-\frac{\hbar^2}{2m_i}\nabla_i^2 + V\right) \exp\left[-\alpha \sum_{i}^{n} \left(x_i^2 + y_i^2 + z_i^2\right)\right] \tag{3}$$

In the simple harmonic oscillator case, this gives:

$$E_L(\mathbf{r}, \alpha) = -\frac{\hbar^2}{2m} \sum_{i=1}^{n} 2\alpha \left(2\alpha(x_i^2 + y_i^2 + z_i^2) - 3\right) + \frac{1}{2} m\omega_{ho}^2 \sum_{i=1}^{n} (x_i^2 + y_i^2 + z_i^2) \tag{4}$$

FIX FOR ONE/N PARTICLES AND LOWER DIMENSION Similarly for the drift force:

$$F = \frac{2\nabla\Psi_T}{\Psi_T} \tag{5}$$

$$F = -2\alpha \sum_{i=1}^{n} (x_i + y_i + z_i) \tag{6}$$

Now for the ugly part:
For one particle, ∇_k:

$$\nabla_k \Psi_T(\mathbf{r}) = \nabla_k \prod_{i=1}^{n} \phi(\mathbf{r}_i) \exp\left(\sum_{i<j} u(r_{ij})\right) \tag{7}$$

Now apply the product rule. For the first term, all terms are unchanged except where $i = k$, giving the first term as:

$$\nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i)\right] \exp\left(\sum_{i<j} u(r_{ij})\right) \tag{8}$$

The second term is trickier. We can rewrite it as follows:

$$\left(\prod_{l} \phi(\mathbf{r_l})\right) \nabla_k \exp\left(\sum_{i=1}^{n}\sum_{i<j} u(r_{ij})\right) = \left(\prod_{l} \phi(\mathbf{r_l})\right) \exp\left(\sum_{i=1}^{n}\sum_{i<j} u(r_{ij})\right) \nabla_k \left(\sum_{i=1}^{n}\sum_{i<j} u(r_{ij})\right) \tag{9}$$

To get anything non-zero in the last term, we must have either $i = k$ or $j = k$. If $i = k$, then the term may be rewritten as:

$$\sum_{k<j} \nabla_k u(r_{kj}) \tag{10}$$

If $j = k$ then all terms such that $i > k$ will vanish, leaving us with:

$$\sum_{i>k} \nabla_k u(r_{ik}) \tag{11}$$

Putting this all together gives:

$$\nabla_k \left(\sum_{i=1}^{n}\sum_{i<j} u(r_{ij})\right) = \sum_{j \neq k} \nabla_k u(r_{ij}) \tag{12}$$