Derivations

Garbage

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Drift Force without interaction

Drift force is given by:

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

With non-interacting particles, we have

$$\Psi_T = \prod_i g(\alpha, \beta, \vec{r}_i)$$

so

$$\nabla g(\alpha, \beta, \vec{r}_i) = \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right) \exp\big(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\big)$$

The partial derivatives are:

$$\begin{aligned}
\frac{\partial}{\partial x} g &= -2\alpha x_i \exp\big(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\big) \\
\frac{\partial}{\partial y} g &= -2\alpha y_i \exp\big(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\big) \\
\frac{\partial}{\partial z} g &= -2\alpha\beta z_i \exp\big(-\alpha(x_i^2 + y_i^2) + \beta z_i^2)\big)
\end{aligned}$$

Using this we find:

$$\nabla g(\alpha, \beta, \vec{r}_i) = -2\alpha(x_i + y_i + \beta z_i) \exp\big(-\alpha(x_i^2 + y_i^2) + \beta z_i^2)\big)$$

Which finally gives:

$$F = \frac{2\nabla g}{g} = -4\alpha \sum_i (x_i + y_i + \beta z_i)$$

1 Local energy without interaction

1.1 Single particle

1.2 N particles

1.2.1 1D

Edit 09.03.18: This is probably wrong. Check. For N particles in one dimension, we have:

$$
\begin{aligned}
\Psi_T &= \prod_i g(\alpha, \vec{r}_i) = \exp\big(-\alpha(x_i^2)\big) \\
E_L &= \frac{\widehat{H}\Psi_T}{\Psi_T} \\
\widehat{H}\Psi_T &= \big(\sum_i \frac{\hbar^2}{2m}\nabla_j^2 + \frac{1}{2}m\omega_{ho}^2 x_i^2\big) \prod_i g_i \\
&= \frac{\hbar^2}{2m}\sum_i \nabla_j^2 \prod_i g_i + \frac{1}{2}m\omega_{ho}^2 x_i^2 \prod_i g_i \\
\nabla_i^2 &= \frac{\partial^2}{\partial x_i^2}
\end{aligned}
$$

Computing the second-derivative of the wave-function:

$$
\begin{aligned}
\nabla_j \prod_i g_i &= \frac{\partial}{\partial x_j}\prod_{i\neq j} g_i = -2\alpha x_i \prod_i g_i \\
\nabla_j^2 \prod_i g_i &= \nabla_j(\nabla_j \prod_i g_i) \\
&= -2\alpha \nabla_j (x_i \prod_i g_i) \\
&= -2\alpha\big(\prod_i g_i + x_i \nabla_j \prod_i g_i\big) \\
&= -2\alpha\big(\prod_i g_i + x_i(-2\alpha x_i \prod_i g_{)}\big) \\
&= 2\alpha \prod_i g_i (2\alpha x_i^2 - 1)
\end{aligned}
$$

With this we find the local energy E_L:

$$E_L = \frac{1}{\prod_i g_i}\big(- \frac{\hbar^2}{2m}\sum_j 2\alpha \prod_i g_i(2\alpha x_i^2 - 1) + \frac{1}{2}m\omega_{ho}^2 \prod_i g_i\big)$$
$$= -\frac{\hbar^2}{m}\alpha N(2\alpha x_i^2 - 2) + \frac{1}{2}m\omega_{ho}^2$$

where $\alpha = \frac{1}{2a_{H_0}^2}$ and $a_{H_0} = \frac{\hbar}{m\omega}$

1.2.2 2D

1.2.3 3D

Edited 08.03.18.

$$\begin{aligned}
\nabla_k \Psi_T(\vec{r}) &= \nabla_k \phi(\vec{r}_k) \cdot \prod_{i\neq k} \phi(\vec{r}_i) \\
\nabla_k^2 \Psi_T(\vec{r}) &= \nabla_k [\nabla_k \Psi_T(\vec{r})] \\
&= \nabla_k [\nabla_k \phi(\vec{r}_k) \cdot \prod_{i\neq k} \phi(\vec{r}_i)] \\
&= \nabla_k^2 \phi(\vec{r}_k) \cdot \prod_{i\neq k} \phi(\vec{r}_i)
\end{aligned}$$

where

$$\begin{aligned}
\nabla_k \phi(\vec{r}_k) &= \nabla_k \exp(-\alpha({x^2}_k + {y^2}_k + \beta {z^2}_k)) \\
&= -2\alpha(x_k + y_k + \beta z_k) \exp(-\alpha({x^2}_k + {y^2}_k + \beta {z^2}_k))
\end{aligned}$$

and

$$\begin{aligned}
\nabla_k^2 \phi(\vec{r}_k) &= \nabla_k\big(\nabla_k \exp(-\alpha({x^2}_k + {y^2}_k + \beta {z^2}_k))\big) \\
&= \nabla_k\big(- 2\alpha(x_k + y_k + \beta z_k) \exp(-\alpha({x^2}_k + {y^2}_k + \beta {z^2}_k))\big) \\
&= -2\alpha\big(\nabla_k(x_k + y_k + \beta z_k) \cdot \exp(-\alpha({x^2}_k + {y^2}_k + \beta {z^2}_k)) \\
&+ \nabla_k \exp(-\alpha({x^2}_k + {y^2}_k + \beta {z^2}_k)) \cdot (x_k + y_k + \beta z_k)\big) \\
&= -2\alpha\big(\nabla_k(x_k + y_k + \beta z_k) \cdot \phi(\vec{r}_k) - 2\alpha(x_k + y_k + \beta z_k)^2 \phi(\vec{r}_k)\big) \\
&= -2\alpha\big((2 + \beta)\phi(\vec{r}_k) - 2\alpha(x_k + y_k + \beta z_k)^2 \phi(\vec{r}_k)\big)
\end{aligned}$$

2 Local energy with interaction

2.1 Note on indices in project file.

The project file has screwed up indices for sums etc in the problem text, and lacks some clarity regarding $f(i,j)$. This is a brief summary of notes made in group session:

$$\begin{aligned}
\phi\vec{r}_i &= \exp(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)) \\
f(r_{ij}) &= \exp(\sum_{i<j} u(r_{ij})) \\
u(r_{ij}) &= ln(f(r_{ij})) = ln(\exp\big(\sum_{i<j} u(r_{ij})\big)) \\
f(r_{ij}) &= \exp\big(u(r_{ij})\big) \\
\nabla_k \exp\big(\sum_{i<j} u(r_{ij}) &= \exp\big(\sum_{i<j} u(r_{ij})\big) \cdot \nabla_k \sum_{l\neq k} u(r_{lk}) \\
\sum_{j\neq k} \nabla_k u(r_{kj})
\end{aligned}$$