Derivations

Garbage

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Drift Force without interaction

Drift force is given by:

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

With non-interacting particles, we have

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

so

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

The partial derivatives are:

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

Using this we find:

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

Which finally gives:

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

1 Local energy without interaction

1.1 Single particle

1.2 N particles

1.2.1 1D

For N particles in one dimension, we have:

$$\Psi_T = \prod_i g(\alpha, \vec{r}_i) = \exp\big(-\alpha(x_i^2)\big)$$

$$E_L = \frac{\widehat{H}\Psi_T}{\Psi_T}$$

$$\widehat{H}\Psi_T = \big(\sum_i \frac{\hbar^2}{2m}\Delta_j^2 + \frac{1}{2}m\omega_{ho}^2 x_i^2\big)\prod_i g_i$$

$$= \frac{\hbar^2}{2m}\sum_i \Delta_j^2 \prod_i g_i + \frac{1}{2}m\omega_{ho}^2 x_i^2 \prod_i g_i$$

$$\Delta_i^2 = \frac{\partial^2}{\partial x_i^2}$$

Computing the second-derivative of the wave-function:

$$\Delta_j \prod_i g_i = \frac{\partial}{\partial x_j}\prod_{i\neq j} g_i = -2\alpha x_i \prod_i g_i$$

$$\Delta_j^2 \prod_i g_i = \Delta_j(\Delta_j \prod_i g_i)$$

$$= -2\alpha \Delta_j (x_i \prod_i g_i)$$

$$= -2\alpha\big(\prod_i g_i + x_i \Delta_j \prod_i g_i\big)$$

$$= -2\alpha\big(\prod_i g_i + x_i(-2\alpha x_i \prod_i g_{)}\big)$$

$$= 2\alpha \prod_i g_i(2\alpha x_i^2 - 1)$$

With this we find the local energy E_L:

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

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

1.2.2 2D

1.2.3 3D

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:

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