

Notes

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Trial wave function

$$\psi(\mathbf{r}) = \psi(\mathbf{r}_1, \dots, \mathbf{r}_N, \alpha, \beta) = \prod_i g(\mathbf{r}_i, \alpha, \beta) \prod_{j < l} f(a, |\mathbf{r}_j - \mathbf{r}_l|)$$

with

$$g(\mathbf{r}_i, \alpha, \beta) = \exp[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)]$$

and

$$f(a, |\mathbf{r}_j - \mathbf{r}_l|) = \begin{cases} 0 & \text{if } |\mathbf{r}_j - \mathbf{r}_l| \leq a \\ 1 - \frac{a}{|\mathbf{r}_j - \mathbf{r}_l|} & \text{if } |\mathbf{r}_j - \mathbf{r}_l| > a. \end{cases}$$

Hamiltonian

$$\sum_i \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{ext}(\mathbf{r}_i) \right) + \sum_{j < k} V_{int}(\mathbf{r}_j, \mathbf{r}_k).$$

In the rest of this notes we are using natural units i.e $\hbar = m = 1$. The local energy is defined as

$$E_L(\mathbf{r}) = \frac{1}{\psi(\mathbf{r})} H \psi(\mathbf{r}).$$

Drift force defined as

$$\mathbf{F} = 2 \frac{\nabla \psi}{\psi}.$$

E_L in 1, 2 and 3 dimensions for N non-interacting particles in harmonic oscillator potentials(**check**).

$$E_{L1}(x) = N\alpha + \sum_i [-2\alpha^2 x_i^2 + V_{ext}(x_i)]$$

$$E_{L2}(\mathbf{r}) = 2N\alpha + \sum_i [-2\alpha^2 \mathbf{r}_i^2 + V_{ext}(\mathbf{r}_i)]$$

$$E_{L3}(\mathbf{r}) = 3N\alpha + \sum_i [-2\alpha^2 \mathbf{r}_i^2 + V_{ext}(\mathbf{r}_i)].$$

Drift force on particle i in non-interacting harmonic potential is

$$\mathbf{F} = -4\alpha\mathbf{r}_i$$

For the full problem we write the wave function as

$$\psi = \prod_i \phi(\mathbf{r}_i) \exp\left(\sum_{j < k} u(r_{jk})\right).$$

With

$$\phi(\mathbf{r}) = g(\alpha, \beta, \mathbf{r}),$$

and

$$u(r_{ij}) = \ln f(a, r_{ij}).$$

Using the product rule and the chain rule one find.

$$\begin{aligned} \nabla_k \psi &= \nabla_k \phi(r_k) \prod_{i \neq k} \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) + \prod_i \phi(r_i) \nabla_k \exp\left(\sum_{j < l} u(r_{jl})\right) \\ &= \nabla_k \phi(r_k) \prod_{i \neq k} \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) + \prod_i \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) \sum_{n \neq k} \nabla_k u(r_{kn}) \end{aligned}$$

Applying the product and chain rule on this one find.

$$\begin{aligned} \nabla_k^2 \psi &= \nabla_k^2 \phi(r_k) \prod_{i \neq k} \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) + 2 \nabla_k \phi(r_k) \prod_{i \neq k} \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) \sum_{n \neq k} \nabla_k u(r_{kn}) \\ &+ \prod_i \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) \sum_{n \neq k} \nabla_k u(r_{kn}) \sum_{l \neq k} \nabla_k u(r_{kl}) + \prod_i \phi(r_i) \exp\left(\sum_{j < l} u(r_{jl})\right) \sum_{n \neq k} \nabla_k^2 u(r_{kn}) \end{aligned}$$

We then get

$$\begin{aligned} \frac{\nabla_k^2 \psi}{\psi} &= \frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)} + 2 \frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j \neq k} \nabla_k u(r_{kj}) \\ &+ \sum_{i \neq k} \sum_{j \neq k} \nabla_k u(r_{ki}) \nabla_k u(r_{kj}) + \sum_{j \neq k} \nabla_k^2 u(r_{kj}) \\ &= \frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)} + 2 \frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j \neq k} \frac{(\mathbf{r}_k - \mathbf{r}_j)}{r_{kj}} u'(r_{kj}) \\ &+ \sum_{i \neq k} \sum_{j \neq k} \frac{(\mathbf{r}_k - \mathbf{r}_i)(\mathbf{r}_k - \mathbf{r}_j)}{r_{ki} r_{kj}} u'(r_{kj}) u'(r_{ki}) \\ &+ \sum_{j \neq k} (u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj})). \end{aligned}$$

Where **(check)**

$$u'(r_{kj}) = \begin{cases} 0 & \text{if } |\mathbf{r}_j - \mathbf{r}_j| \leq a \\ a(r_{kj}^2 - ar_{kj})^{-1} & \text{if } |\mathbf{r}_j - \mathbf{r}_j| > a. \end{cases}$$

$$u''(r_{kj}) = \begin{cases} 0 & \text{if } |\mathbf{r}_j - \mathbf{r}_j| \leq a \\ \frac{a^2 - 2ar_{kj}}{(r_{kj}^2 - ar_{kj})^2} & \text{if } |\mathbf{r}_j - \mathbf{r}_j| > a. \end{cases}$$

$$\frac{\nabla_k \phi(r_k)}{\phi(r_k)} = -2\alpha(x\hat{x} + y\hat{y} + \beta z\hat{z})$$

$$\frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)} = -2\alpha((2 + \beta) - 2\alpha(x^2 + y^2 + \beta z^2))$$

References