Notes

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Trial wave function

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

with

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

and

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

Hamiltonian

$$\sum_i (-\frac{\bar{h}^2}{2m}\nabla_i^2 + V_{ext}(\boldsymbol{r}_i)) + \sum_{j<k} V_{int}(\boldsymbol{r}_j, \boldsymbol{r}_k).$$

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

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

Drift force defined as

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

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

$$E_{L1}(x) = \sum_i [\alpha(1 - 2\alpha x_i^2) + V_{ext}(x_i^2)]$$

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

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

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

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

For the full problem we writhe the wave function as

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

With

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

and

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

Using the product rule and the chain rule one find.

$$\nabla_k \psi = \nabla_k \phi(r_k) \prod_{i \neq k} \phi(r_i) exp\big(\sum_{j<l} u(r_{jl})\big) + \prod_i \phi(\boldsymbol{r}_i) \nabla_k exp\big(\sum_{j<l} u(r_{jl})\big)$$

$$= \nabla_k \phi(r_k) \prod_{i \neq k} \phi(r_i) exp\big(\sum_{j<l} u(r_{jl})\big) + \prod_i \phi(\boldsymbol{r}_i) exp\big(\sum_{j<l} u(r_{jl})\big) \sum_{n \neq k} \nabla_k u(r_{kn})$$

Applying the product and chain rule on this one find.

$$\nabla_k^2 \psi = \nabla_k^2 \phi(r_k) \prod_{i \neq k} \phi(r_i) exp\big(\sum_{j<l} u(r_{jl})\big) + 2\nabla_k \phi(r_k) \prod_{i \neq k} \phi(\boldsymbol{r}_i) exp\big(\sum_{j<l} u(r_{jl})\big) \sum_{n \neq k} \nabla_k u(r_{kn})$$

$$+ \prod_i \phi(\boldsymbol{r}_i) exp\big(\sum_{j<l} u(r_{jl})\big) \sum_{n \neq k} \nabla_k u(r_{kn}) \sum_{l \neq k} \nabla_k u(r_{kl}) + \prod_i \phi(\boldsymbol{r}_i) exp\big(\sum_{j<l} u(r_{jl})\big) \sum_{n \neq k} \nabla_k^2 u(r_{kn})$$

We then get

$$\frac{\nabla_k^2 \psi}{\psi} = \frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)} + 2 \frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j \neq k} \nabla_k u(r_{kj})$$

$$+ \sum_{i \neq k} \sum_{j \neq k} \nabla_k u(r_{ki}) \nabla_k u(r_{kj}) + \sum_{j \neq k} \nabla_k^2 u(r_{kj})$$

$$= \frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)} + 2 \frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j \neq k} \frac{(\boldsymbol{r_k} - \boldsymbol{r_j})}{r_{kj]}} u'(r_{kj})$$

$$+ \sum_{i \neq k} \sum_{j \neq k} \frac{(\boldsymbol{r_k} - \boldsymbol{r_i})(\boldsymbol{r_k} - \boldsymbol{r_j})}{r_{ki} r_{kj}} u'(r_{kj}) u'(ki)$$

$$+ \sum_{j \neq k} (u''(r_{kj}) - \frac{2}{r_{kj}} u'(r_{kj})).$$

Where(**check**)

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

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

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

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

References