FYS 4411/9411

Computational Physics 2

FYS4411

Basics of MC (VMC) calculation

- need a trial wave function (wf)

- need a Hamiltonian.

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

onebody operator (non-interacting part)

interacting part (two-body three-body ---

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$$\hat{H}_0 = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + \hat{v}_{ext}(\vec{r}_i) \right)$$

number of particles

$$\hat{v}_{ext} = \frac{1}{2} m \omega^2 r_i^2$$

$$r_i^2 = (x_i^2 + y_i^2 + z_i^2)$$

For one single particle we have an analytical for the harmonic oscillator.

1-Dim ground state

$$\left(-\frac{\hbar^2}{2m} D^2 + \frac{1}{2} m \omega x^2 \right) \psi(x) = \varepsilon_0 \psi(x)$$

$$D^2 = \frac{d^2}{dx^2}$$

$$\varepsilon_0 = \hbar \omega (n_x + 1) 1/2$$

$$n_x = 0 \Rightarrow \varepsilon_0 = \frac{1}{2} \hbar \omega$$

$\psi(x) \Rightarrow \psi_0(x) = \alpha\, e^{-\frac{1}{2}\omega^2 x^2}$

$\psi_0(x) \sim e^{-\frac{1}{2}\beta x^2}$

2 Dim $\quad n_x = n_y = 0$

$E_0 = \hbar\omega$

$\psi_0(x) \sim e^{-\frac{1}{2}\beta(x^2+y^2)}$

3 Dim $\quad n_x = n_y = n_z = 0$

$E_0 = 3/2\,\hbar\omega$

$\psi_0(x) \sim e^{-\frac{1}{2}\beta(x^2+y^2+z^2)}$

d- Dim

$$E_0 = \frac{d}{2}\hbar\omega$$

$\psi_0(x) \sim e^{-\frac{1}{2}\beta r^2}$

$$r^2 = \sum_{i=1}^{d} x_i^2$$

general coordinate.

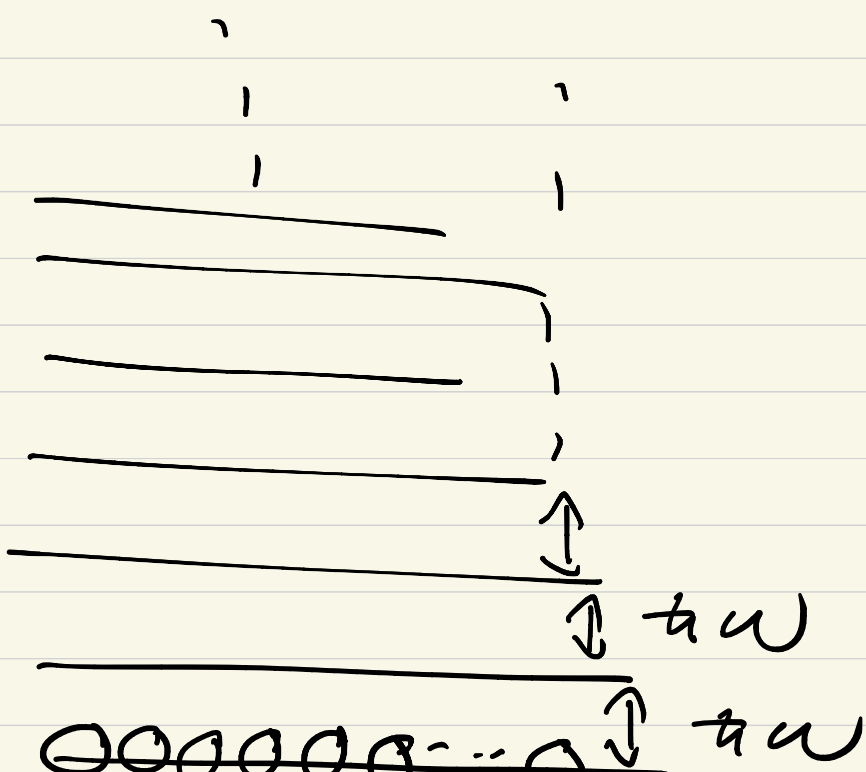
Ansatz for non-interacting Bosons

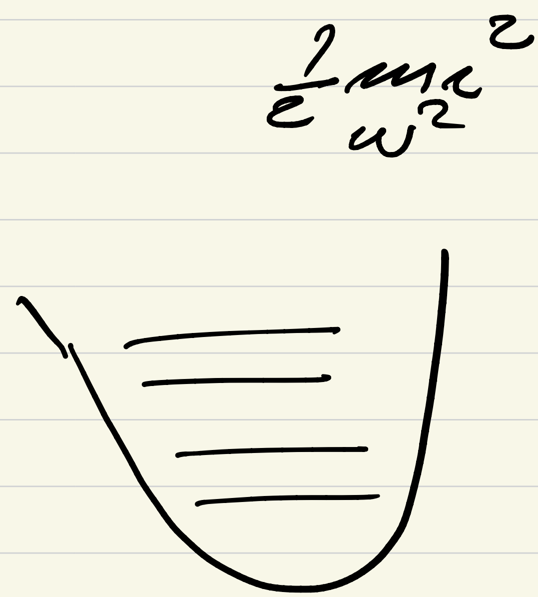
$$\Psi_0(\vec r_1, \vec r_2, \vec r_3, \dots, \vec r_N) = \prod_{i=1}^{N} e^{-\frac{1}{2}\beta r_i^2}$$

analytical

$$\hat H_0 \Psi_0 = E_0 \Psi_0$$

$$= \boxed{N \cdot \frac{d}{2} \hbar\omega}$$





VMC approach;

Basic element we want to evaluate

$$\mathbb{E}[H] = \frac{\int d\vec{r}\, \Psi_T^* \hat{H} \Psi_T}{\int d\vec{r}\, \Psi_T^* \Psi_T}$$

$$d\vec{r} = d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 \cdots d\vec{r}_N$$

$$\Psi_T = \Psi_T(\vec{r}; \vec{\beta})$$

quantum numbers

variational parameters

$$\min_{\vec{\beta}} \mathbb{E}[H]$$

How can we evaluate $\mathbb{E}[H]$ as a function of $\vec{\beta}$?

We want to rewrite in terms of

$$\int d\tilde{r}\, P\, E$$

PDF

$$\mathbb{E}[A] = \int d\tilde{r}\, P(\vec{r}, \vec{\beta})\, A(\tilde{r}, \ldots)$$

<u>Define</u> $P(\vec{r}; \vec{\beta})$

$$= \frac{|\Psi_T(\vec{r}; \vec{\beta})|^2}{\int d\vec{r}\, |\Psi_T(\vec{r}; \beta)|^2}$$

Define the local energy

$$E_L(\vec{r}; \vec{\beta}) = \frac{1}{\Psi_T} \hat{H} \Psi_T$$

$$\mathbb{E}[H] = \frac{\int d\tilde{r}\, \Psi_T^* H \Psi_T}{\int d\tilde{r}\, |\Psi_T|^2}$$

$$\mathbb{E}[H] = \mathbb{E}[E_L(\vec{\beta})] =$$

$$\int d\vec{r}\, P(\vec{r};\vec{\beta})\, E_L(\vec{r};\vec{\beta})$$

$$\simeq \frac{1}{M} \sum_{i=1}^{M} E_L(\vec{r}_i;\vec{\beta})$$

\# Monte Carlo samples

= Randomly selected positions $\vec{r}_i = (\vec{r}_1^{(i)}, r_2^{(i)}, \ldots r_N^{(i)})$

Ingredients in VMC

$$E_L = \frac{1}{\Psi_T} \hat{H} \Psi_T$$

$$= \frac{1}{\Psi_T} \left[\sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + \hat{V}_{ext}(\vec{r}_i) \right) + H_I \right) \times \Psi_T$$

1)

$$\boxed{\frac{1}{\psi_T}\left[\sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2\right]\psi_T}$$

First one is $\psi_T =$

$$\prod_{i=1}^{N} e^{-\frac{1}{2}\beta r_i^2}$$

2)

$$\frac{1}{\psi_T}\left[\sum_{i=1}^{N} \frac{1}{2}m\omega^2 r_i^2\right]\psi_T$$

V^{Ext}

$$= \sum_{i=1}^{N} \frac{1}{2}m\omega^2 r_i^2$$

3)

$$\frac{1}{\psi_T}\hat{H}_1\psi_T = H_1$$

$$\left(H_1 = \sum_{i<j}^{N} v(|\vec{r}_i - \vec{r}_j|) \right)$$

END JAN 16 LECTURE, 2020

Kinetic energy

$$\langle T \rangle \simeq \frac{1}{M} \sum_{i=1}^{M} \frac{1}{\psi_T(\vec{r}_i)} \left(\sum_{j=1}^{N} -\frac{\hbar^2}{2m} \nabla_j^2 \psi_T(\vec{r}_i) \right)$$

From a single particle j

$$\frac{1}{\psi_T} \; -\frac{\hbar^2}{2m} \nabla_j^2 \psi_T(\vec{r}_1^{\,i}, \vec{r}_2^{\,i}, \ldots \vec{r}_j^{\,i} \ldots \vec{r}_N^{\,i})$$

- Numerically

$$\frac{d^2 u(x)}{dx^2} \simeq \frac{u(x+\Delta x) + u(x-\Delta x) - 2u(x)}{(\Delta x)^2}$$

In three/two dims

$$\frac{d^2 u(x,y,z)}{dx^2} =$$

$$u(x,y,z) \to u(x_i, y_j, z_k)$$

$$= u_{ijk}$$

$$u(\underset{\overset{\parallel}{h}}{x+\Delta x}, y, z) = u_{i+1jk}$$

1) $$\frac{d^2u}{dx^2} = \frac{u_{i+1jk} + u_{i-1jk} - 2u_{ijk}}{h^2}$$

2) $$\frac{d^2u}{dy^2} = \frac{u_{ij+1k} + u_{ij-1k} - 2u_{ijk}}{h^2}$$

reset $x_i + h \rightarrow x_i$

$x_i - h \rightarrow x_i$

$u_{i+1j+1k}$ instead of u_{ij+1k}

- Numerical approach is useful to benchmark the analytical result?

- Numerical approach if it is too complicated to set up analytical expressions with given eq

3) For our case

$$\Psi_T = \prod_{i=1}^{N} e^{-\alpha r_i^2} \times \prod_{i<j} f(r_{ij})$$

single-particle part

$r_{ij} = |\vec{r}_i - \vec{r}_j|$ central force

Correlated part / Correlation part / Jastrow / Jastrow-Padé

- - - -

Pain + difficulty with the analytical expression for E_L.

VMC code

$$\langle E \rangle = \mathbb{E}[E_L]_{\vec{\alpha}} \simeq \frac{1}{M}\sum_{i=1}^{M} E_L(\vec{r}_i;\vec{\alpha})$$

variance $\sigma_E^2 = \mathbb{E}[(E_L - \langle E \rangle)^2]$

need $\langle E^2 \rangle$

$\sigma_E^2 = 0$

$\langle E \rangle$ = unknown
don't know the exact value

if $\psi_T = \psi_{Exact}$

$$\sigma_E^2 = \frac{\int \psi_T^* \hat{H}^2 \psi_T \, d\vec{r}}{N} - \left[\frac{\int \psi_T^* \hat{H} \psi_T \, d\vec{r}}{N}\right]^2$$

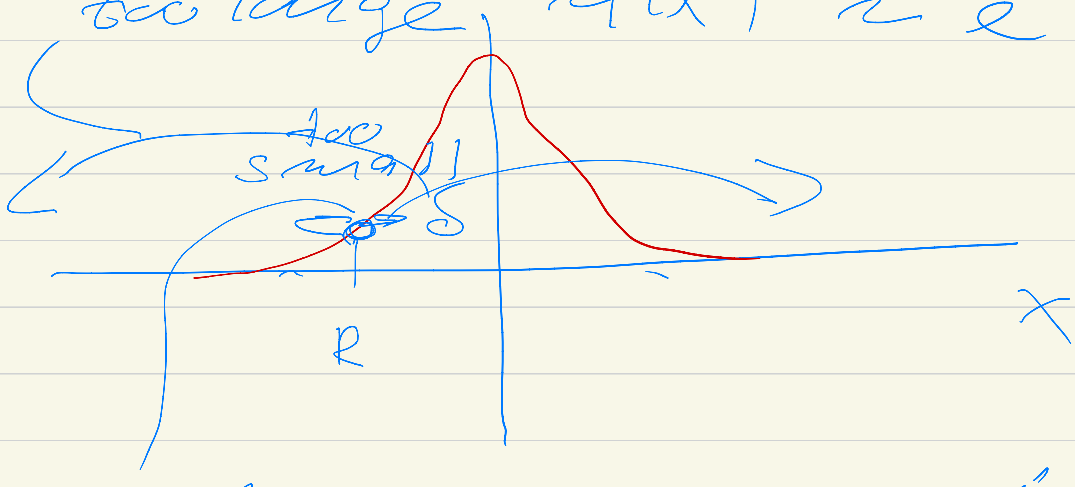
$$\langle E^2 \rangle - \langle E \rangle^2$$

$$\hat{H}\psi_{Exact} = E_{Exact}\psi_{Exact}$$

We want $E[E_L(\Psi_T)]$ which as close as possible to the Exact energy (unknown) and $\sigma_E^2 \to 0$

Harmonic oscillator 1-dim

$\Psi(x) \sim e^{-\frac{1}{2}\alpha^2 x^2}$



when jumping in space (picking different configuration/samples) we make a proposal

$R' = R + r\delta$

$r \in [-0.5, +0.5]$

$\delta \to$ has to be tuned by you?

Trial wf $\psi_T(r_1, r_2, \ldots r_N; \alpha)$

$$= \prod_{i=1}^{N} e^{-\frac{1}{2}\alpha^2 r_i^2}$$

1-Dim $\quad r_i^2 = x_i^2$

2-dim $\quad r_i^2 = x_i^2 + y_i^2$

3-dim $\quad r_i^2 = x_i^2 + y_i^2 + z_i^2$

Harmonic oscillator in 1-dim

$$u(x) = \boxed{x R(x)} \quad \Big| \quad u(r) = r R(r)$$

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dx^2} + \frac{1}{2} m \omega^2 x^2 u(x)$$

$$= E\, u(x) \qquad u(x) \sim \boxed{\alpha x\, e^{-\frac{1}{2}\alpha^2 x^2}}$$

Scale equations

$$x = \gamma \rho \qquad [\rho] = \text{no dim}$$

$$[\gamma] = \text{length}$$

$$-\frac{\hbar^2}{2\gamma^2 m}\frac{d^2 u}{d\rho^2} + \frac{1}{2} m \omega^2 \gamma^2 \rho^2 u$$

$$\times \frac{\gamma^2 m}{\hbar^2} \qquad\qquad = E u$$

$$-\frac{1}{2}\frac{d^2u}{d\xi^2} + \frac{1}{2}\frac{m^2\gamma^4}{\hbar^2}\xi^2\omega^2 u$$

$$= \lambda u$$

$$\lambda = \frac{m^2\gamma^2}{\hbar^2}E$$

$$\frac{m^2\gamma^4}{\hbar^2}\omega^2 = \underline{1} \quad \Rightarrow$$

$$\gamma = \sqrt{\frac{\hbar\,\hbar\,c^2}{m\omega\hbar c^2}}$$

Natural length scale in terms of the physical constants

$$\hbar = c = e = m = \underline{1}$$

choose $\omega = \underline{1}$

$$\gamma = \underline{1}$$

Metropolis algorithm

Most likely PDF : P_i

Markov chain

$$P_i(t+\varepsilon) = \sum_j W(j \to i)\, P_j(t)$$

$$P_i^{(n)} = \sum_j W(j \to i)\, P_j^{(n-1)}$$

II steps

Transition probability

We have a model for

$$P_i^{(n)} = \frac{|\psi_i|^2}{\int |\psi_i|^2 d\tau}$$

multidimensional

$W(j \to i)$ = unknown

We can model W

$$W(j \to i) = A(j \to i)\, \underline{T(j \to i)}$$

acceptance of proposed move

The likelihood for a specific transition

Modified Metropolis algorithm $\Rightarrow$

Metropolis Hastings algo,

Metropolis (Brute force)

$$T(j \to i) = T(i \to j)$$

Detailed balance

$$\frac{P_i}{P_j} = \frac{W(j \to i)}{W(i \to j)}$$

known

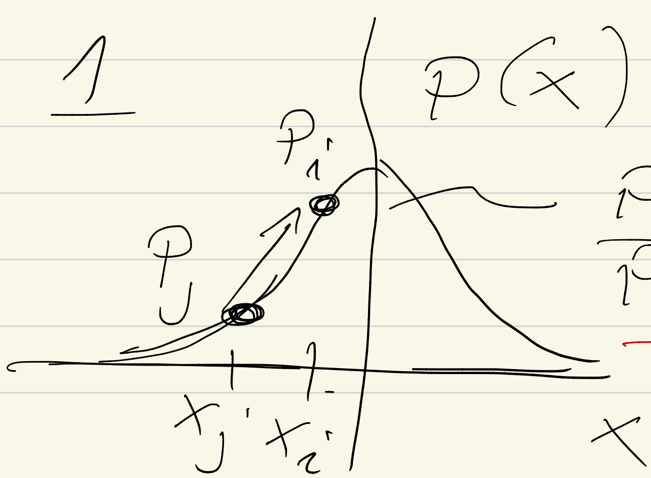
$$= \frac{A(j \to i)\,\cancel{T(j \to i)}}{A(i \to j)\,\cancel{T(i \to j)}}$$

$$= \frac{A(j \to i)}{A(i \to j)}$$

unknown

$$0 \le A(i \to i) \le 1$$

$$\frac{P_i}{P_j} > 1$$



$$\frac{P_i}{P_j} > 1$$

$$\boxed{A(j \to i) = 1}$$

$$A(i \to j) < 1$$

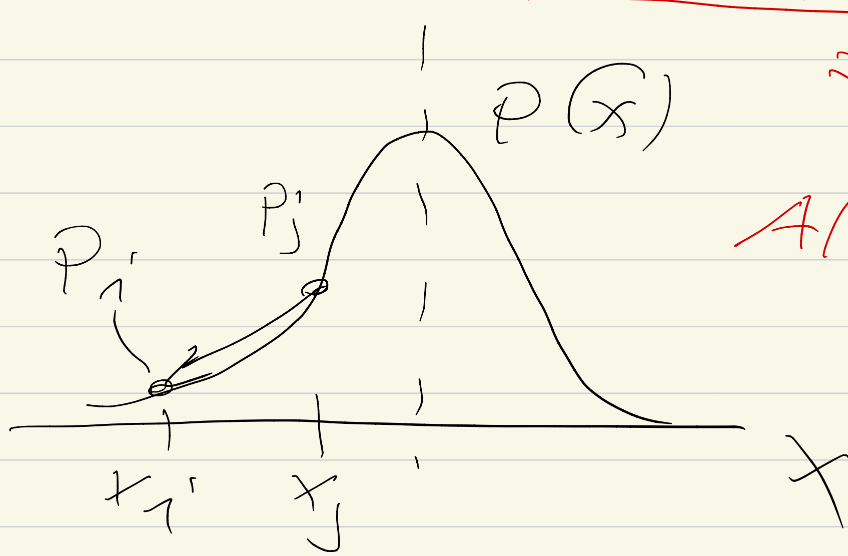
$$\frac{A(j \to i)}{A(i \to j)} > 1$$

$$\frac{A(j \to i)}{A(i \to j)} = 1$$, stay at the same place

$$\frac{P_i}{P_j} < 1 \Rightarrow \frac{A(j \to i)}{\boxed{A(i \to j)}} < 1$$

$= 1$

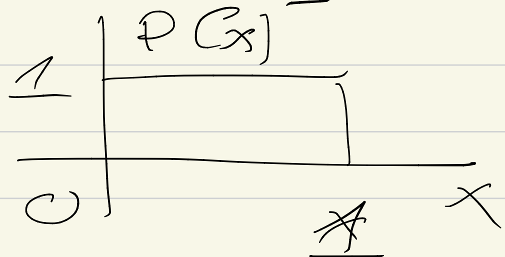
$A(j \to i) < 1$



Metropolis algo

$$A(j \to i) = \min\left(1, \frac{p_i}{p_j}\right)$$

compute a random number $r \in [0,1]$
(uniform PDF



accept move if

$$\boxed{r \le p_i / p_j}$$

$$T(j \to i) = T(i \to j)$$

if not

$$A(j \to i) = \min\left(1, \frac{p_i \, T(i \to j)}{p_j \, T(j \to i)}\right)$$

Need a model

How do we model $T(i \to j)$? $\Rightarrow$ Importance sampling.

$$T(i \to j) = T \Rightarrow T(t, \vec{x})$$

use Fokker-Planck eq.

$$\boxed{\frac{\partial T}{\partial t} = D \frac{\partial^2}{\partial x^2} T(x,t)} - D \frac{\partial}{\partial x} F\, T(x,t)$$

standard Diffusion equation.

Drift force

$$F = F(x)$$

$$\frac{\partial T}{\partial t} = \sum_i D \vec{e}_i \frac{\partial}{\partial x_i} \left(\vec{e}_i \frac{\partial}{\partial x_i} - \vec{F}_i \right) \times T(\vec{x}, t)$$

The convergence towards a stationary state (equilibrium, most likely state)

$$\frac{\partial T}{\partial t} = 0 =$$

$$\sum_i D \, \vec{e}_i \frac{\partial}{\partial x_i} \left(\vec{e}_i \frac{\partial}{\partial x_i} - \vec{F}_i \right) T$$

zero if

$$\underline{\frac{\partial^2 T}{\partial x_i^2}} = T \frac{\partial}{\partial x_i} F_i +$$

$$F_i \frac{\partial}{\partial x_i} T$$

$$\underline{F} = g(x) \frac{\partial T}{\partial x}$$

$$\frac{\partial^2 T}{\partial x_r^2} = T \frac{\partial g}{\partial x_r} \left(\frac{\partial T}{\partial x_r} \right)^2 + T g \frac{\partial^2 T}{\partial x_r^2} + g \left(\frac{\partial T}{\partial x_r} \right)^2$$

Terms containing first and second derivatives have to cancel each other. Only possible if

$$g = \frac{1}{T}$$

$$\Rightarrow \quad \vec{F} = 2 \frac{1}{\psi_T} \vec{\nabla} \psi_T$$

✓ named quantum force.

The solution to the Fokker-Planck equation

$$\frac{\partial T}{\partial t} = \sum_i D \frac{\partial}{\partial x_i}\left(\frac{\partial}{\partial x_i} - F_i\right) T(x,t)$$

$\simeq \frac{1}{\psi_T} D \psi_T$

Δt

$T(y, x, t) =$

state i state j

$$\frac{1}{(4\pi D \Delta t)} \exp\left(-\frac{(y - x - D\Delta t F(x))^2}{4 D \Delta t}\right)$$

parameter

Metropolis-Hastings

$$A(x \to y) = \frac{T(x \to y)\,|\psi_T(y)|^2}{T(y \to x)\,|\psi_T(x)|^2}$$

- computational aspects

$$\psi_T = \psi_{OB}\,\psi_C$$

one-body

correlated part

$$\prod_{i=1}^{N} e^{-\alpha^2 r_i^2}$$

$$\prod_{i<j} g(r_{ij})$$

$$r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}$$

$$r_{ij} = |\vec{r}_i - \vec{r}_j|$$

$$\exp\left\{\sum_{i<j} f(r_{ij})\right\}$$

Two particles interacting via a Coulomb force

$$\prod_{i<j} g(r_{ij}) = \exp\left\{ \pm \frac{r_{12}}{1+\beta r_{12}+\dots} \right\}$$

r_{12}

Ratio in Metropoli's Test (without Importance sampling)

① $$\frac{|\Psi_T^{new}|^2}{|\Psi_T^{old}|^2} = \frac{|\Psi_{OB}^{new}|^2 |\Psi_C^{new}|^2}{|\Psi_{OB}^{old}|^2 |\Psi_C^{old}|^2}$$

② quantum force

$$\frac{\nabla \Psi_T}{\Psi_T} = \frac{\nabla(\Psi_{OB}\Psi_C)}{\Psi_{OB}\Psi_C}$$

$$= \frac{\nabla \psi_{OB}}{\psi_{OB}} + \frac{\nabla \psi_C}{\psi_C}$$

two particles

$$\frac{1}{\psi_{OB}} \sum_{i=1}^{2} \vec{\nabla}_i \psi_{OB}$$

$$\psi_{OB} = e^{-\alpha^2 (r_1^2 + r_2^2)}$$

$$= e^{-\alpha^2 (x_1^2 + x_2^2)}$$

$$\frac{e^{-\alpha^2 (x_1^2 + x_2^2)} \left[-\alpha^2 2 x_1 - \alpha^2 2 x_2 \right]}{e^{-\alpha^2 (x_1^2 + x_1^2)}}$$

gradient

$$\boxed{= -\alpha^2 2 x_1 - \alpha^2 2 x_2}$$

3

$$\langle K_i \rangle = -\frac{1}{2} \frac{\langle \psi_T | \nabla_i^2 | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

in the local energy we need

$$\hat{K}_i = -\frac{1}{2}\frac{1}{\psi_T}\nabla_i^2\psi_T$$

$$\frac{\nabla^2\psi_T}{\psi_T} = \frac{\nabla^2\psi_{0B}}{\psi_{0B}} + \frac{\nabla^2\psi_C}{\psi_C} + 2\,\frac{\vec{\nabla}\psi_{0B}}{\psi_{0B}}\cdot\frac{\vec{\nabla}\psi_C}{\psi_C}$$

product of two gradients