FYS4411/9411 Comp Phys 2/Jan 27

Ingredients needed to build a VMC program

$$\mathbb{E}[H] = \langle E[\vec{\alpha}] \rangle$$

$$(= \bar{E}[\alpha])$$

$$= \frac{\int_{\vec{R}\in D} d\vec{R}\, \psi_T^*(\vec{R};\vec{\alpha}) \frac{\psi_T}{\psi_T} H(\vec{R})\, \psi_T(\vec{R};\vec{\alpha})}{\int d\vec{R}\, |\psi_T(\vec{R};\vec{\alpha})|^2}$$

Define a PDF

$$P_T(\vec{R};\vec{\alpha}) = \frac{|\psi_T(\vec{R};\vec{\alpha})|^2}{\int_{\vec{R}\in D} d\vec{R}\, |\psi_T(\vec{R};\vec{\alpha})|^2}$$

Local energy

$$E_L(\vec{R};\vec{\alpha}) = \frac{1}{\psi_T(\vec{R};\vec{\alpha})} H(\vec{R})\, \psi_T(\vec{R};\vec{\alpha})$$

$$\vec{\alpha} = [\alpha_1, \alpha_2, \alpha_3, \ldots \alpha_m]$$

$$\mathbb{E}[H] = \mathbb{E}[E_L[\vec{\alpha}]]$$

$$= \langle E_L[\vec{\alpha}] \rangle = \int_{\vec{R} \in D} d\vec{R} \; P_T(\vec{R}; \vec{\alpha}) \times E_L(\vec{R}; \vec{\alpha})$$

Define $\psi_T(\vec{R}; \vec{\alpha})$

— " — $H(\vec{R})$

— " — E_L, P_T

How to build a program

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system

wave (trial) functions

local energy

Hamiltonian if possible analytical

Solver

- Markov-chain MC $(MC)^2$
- sampling
  - Metropolis
  - [illegible]

expression for E_L, Ψ_T and their derivatives

- Evaluate errors
  - Resampling methods
    - Bootstrap
    - Jackknife
    - Blocking
- optimal parameters $\alpha_i \quad i=1,2,\ldots m$

$$\frac{\partial \langle E_L(\vec{\alpha})\rangle}{\partial \alpha_i} = 0$$

  - gradient methods
- High-performance computing
  - MPI
  - OPEN MP
- Neural Networks
- other many-body

1-Dim ho potential

Schrödinger's equation

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

$$= \varepsilon\,\psi(x)$$

$$\varepsilon_n = \hbar\omega(n + 1/2) \quad n = 0, 1, 2, \ldots$$

Scale equations

Dim less length $\quad \rho = \gamma \cdot x$

$$x = \rho/\gamma$$

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

$$\times\,\psi(\rho) = \varepsilon\,\psi(\rho)$$

$$\times\ \frac{m}{\hbar^2\gamma^2}$$

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

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

$$\gamma^2 = \frac{\hbar}{m\cdot\omega} \Rightarrow$$

$$\gamma = \sqrt{\frac{\hbar}{m\omega}}$$

natural length scale

natural units

$$c = \hbar = m = 1$$

Trial wf :

$$\psi_T(x;\alpha) = e^{-\frac{1}{2}\alpha^2 x^2}$$

$$E_2 = \frac{1}{\psi_T}\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right)\psi_T$$

$$\xi \to x$$

$$= \frac{1}{2}\left(\alpha^2 + x^2(1-\alpha^4)\right)$$

$$\langle E_L[\alpha] \rangle = \int_{-\infty}^{\infty} dx \, P_T(x;\alpha) E_L(x;\alpha)$$

$$= \frac{\int_{-\infty}^{\infty} dx \, e^{-\alpha^2 x^2} \frac{1}{2}\left(\alpha^2 + x^2(1-\alpha^4)\right)}{\int_{-\infty}^{\infty} dx \, e^{-\alpha^2 x^2}}$$

$$= \frac{1}{4}\left(\alpha^2 + \frac{1}{\alpha^2}\right)$$

optimal α

$$\frac{d \langle E_L[\alpha] \rangle}{d\alpha} = 0$$

$$= \frac{1}{2}\alpha - \frac{1}{2\alpha^3} \Rightarrow$$

$$\underline{\underline{\alpha = 1}}$$

$$\langle E_L[\alpha = 1] \rangle = \frac{1}{\ }$$

$\hbar = c = m = \underline{1}^{2} \quad (\omega = 1)$

normally we don't know ψ_{Exact}. How can we judge from $\psi_T(x;\alpha)$ whether we are close or equal to ψ_{Exact}?

variance defined as

$$\sigma_x^2 = \int_{x\in D} x^2 p(x)\,dx - \Big[\underbrace{\int_{x\in D} x\,p(x)\,dx}_{=\mu_x}\Big]^2$$

$$\mathbb{E}[H^2] = \frac{\int_{x\in D} \psi^*(x) H^2 \psi(x)\,dx}{\int dx\, |\psi|^2}$$

$H\psi(x) = \varepsilon\,\psi(x)$; exact solution if $\psi_T = \psi_{exact}$

$$\mathbb{E}[H^2] = \varepsilon^2 \frac{\int |\psi|^2 dx}{\int |\psi|^2 dx}$$

$$= \varepsilon^2$$

$$(\mathbb{E}[H])^2 = \varepsilon^2$$

$$\sigma_H^2 = \mathbb{E}[H^2] - [\mathbb{E}[H]]^2$$

$$= 0 \quad \text{if } \psi_T = \psi_{exact}.$$

$$\psi_T(x;\alpha) = e^{-\frac{1}{2}\alpha^2 x^2}$$

$$\sigma^2[\alpha] = \frac{1}{4}\left(1 + (1-\alpha^2)\frac{3}{4\alpha^2}\right)$$

$$- \langle E_L[\alpha] \rangle^2$$

$\alpha = \underline{1}$

$$\sigma^2[\alpha] = \frac{1}{4} - \left(\frac{1}{2}\right)^2 \equiv 0$$

How to find ψ_T?

Hydrogen atom

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{ke^2}{r}\right)\psi(\vec{r}) = \varepsilon\,\psi(\vec{r})$$

$x, y, z \Rightarrow r, \theta, \varphi$

$r \in [0, \infty)$

Diff eq. for r

$$\left(-\frac{\hbar^2}{2m}\frac{d}{dr}r\frac{d}{dr} + \frac{\ell(\ell+1)\hbar^2}{r^2} - \frac{ke^2}{r}\right)R(r) = E_r R(r)$$

$\ell = 0$, $\hbar = 1 = e = c = m$

$$E_L(r) = \frac{1}{R(r)}\left(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} - \frac{1}{r}\right)R(r)$$

$r \Rightarrow 0$ divergence

in $-\frac{2}{r}\frac{d}{dr}$ and $-\frac{1}{r}$

$$\lim_{r \to 0} \frac{d^n \psi(r)}{d r^n} = \text{constant}$$

$$\lim_{r \to 0} E_L(r) = \frac{1}{R}\left(-\frac{2}{r}\frac{dR}{dr} - \frac{1}{2}R\right) = 0$$

$$-\frac{2}{R\cancel{r}}\frac{d}{dr}R - \frac{1}{\cancel{r}} \Rightarrow$$

$$\frac{dR}{dr} = -\frac{1}{2}R$$

$$R(r) = e^{-\frac{1}{2}r} \Rightarrow$$

$$\psi_T(r;\alpha) = e^{-\alpha \cdot r}$$