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جلسه ۲۳ر۹ر۱۴۰۰

Variational Quantum Monte Carlo

① Time Independent Shrodinger Eq.

$$E(\{\theta\}) = \int d\underbrace{\vec{R}}_{\text{مختصات ذرات سیستم}} \, \overbrace{\underbrace{P(\{\theta\},\vec{R})}_{\text{Trial/guide wavefunction}}}^{\text{Von\_Neumann}} \, E_L(\{\theta\},\vec{R})$$

Trial/guide wavefunction

The Coordinates of particle

$$E(\{\theta\}) = \frac{1}{N} \sum_{i=1}^{N} E_L(\{\theta\}, \underbrace{\vec{R}_i}_{})$$

Some Comments on Computing Local Energy

$$\boxed{E_L(\{\theta\},R) = \frac{\mathcal{H}\,\Psi_T(\{\theta\},\vec{R})}{\Psi_T(\{\theta\},\vec{R})}}$$

$$\mathcal{H} = \mathcal{H}_{\text{Kinetic}} + \mathcal{H}_{\text{Intraction}} = \underbrace{\sum_{i=1}^{N} \mathcal{H}_{K}^{(i)}} + \underbrace{{\sum_{ij}}' \mathcal{H}_{Int}^{(ij)}}$$

$$E_L(\{\theta\}, R) = E_L^{\text{Kinetic}} + E_L^{\text{Intracti}}$$

$$\rightarrow E_L^{\text{Kinetic}} = \frac{\mathcal{H}_{\text{Kinetic}}\, \psi_T(\{\theta\}, \vec{R})}{\psi_T(\{\theta\}, \vec{R})}$$

{ Many-Particle Wave functi }

To Remind you.

$\rightarrow$ $\overbrace{\text{Classical System}}^{\text{Maxwell-Boltzmann}}$

$\rightarrow$ $\overbrace{\text{Bosonic System}}^{\text{BE Distributi}}$

$\rightarrow$ FD Distri
Fermionic System

$$\rightarrow \psi_N^{\text{class.}}(\vec{R}) = \prod_{i=1}^{N} \psi_i^{(1)}(\vec{R}) \rightarrow$$

یک سیستم کلاسیک بن ذره

Many-Body Wave functi

تمیزپذیر هستند

for Distinguishable

(Partn

$$\psi_N^{BE}(R) = \psi_N^{\text{Symmetric}}(R) = \sum_p \hat{p}\, \psi_N^{\text{class}}$$

N=2 $$\psi_2^{BE} = \frac{\left[\psi_1^{\text{clas}}(\vec{R}_1)\, \psi_2^{\text{clas}}(\vec{R}_2) + \psi_1^{\text{clas}}(R_2)\, \psi_2^{\text{clas}}(R_1)\right.}{\sqrt{2}}$$

$$\psi_N^{FD}(R) = C^{ts} \sum_p \delta_p\, \hat{p}\, \psi_N^{\text{class}}$$

$$\delta_p = \begin{cases} +1 & \text{even Permutation} \\ -1 & \text{odd Permutation} \end{cases}$$

$\psi_N^{FD}(\bar{R}) \equiv$ Slater determinant

N=2 $$\psi_2^{FD}(\vec{R}) = \begin{vmatrix} \psi_1(R_1) & \psi_2(R_1) \\ \psi_1(R_2) & \psi_2(R_2) \end{vmatrix}$$

$$= \frac{\psi_1(\vec{R}_1)\, \psi_2(R_2) - \psi_1(R_2)\, \psi_2(R_1)}{\sqrt{2}}$$

$$E_L^{Kinetic}(\{\theta\}, \vec{R}) = ?$$

$$E_L^{Kinet}(\{\theta\}, \vec{R}_{i}) = \frac{\mathcal{H}^{(i)}_{Kin} \Psi_T(\{\theta\}, \vec{R})}{\Psi_T(\{\theta\}, \vec{R})}$$

نمونه‌ام سیستم

$$= -\frac{\hbar^2}{2m} \frac{\nabla_i^2 \Psi_T(\{\theta\}, \vec{R})}{\Psi_T(\{\theta\}, \vec{R})}$$

مشتق نسبت به موقعیت ذره‌ام.

Positive Pos

$$\rightarrow E_L^{Kinet\,(i)} = 2T_i - |F_i|^2$$

$$\rightarrow T_i \equiv -\frac{\hbar^2}{4m} \nabla_i^2 \ln|\Psi_T(\{\theta\}, \vec{R})|$$

$$\rightarrow F_i \equiv \frac{\hbar}{\sqrt{2m}} \vec{\nabla}_i \ln|\Psi_T(\{\theta\}, \vec{R})|$$

$$\lim_{N\to\infty} \langle |F_i|^2 \rangle = T_i$$

# of Run

" if we Use above Parts to Compute"

Local Energy. It can be shown

that, this for may have better

behavior to Convergen to

expected local Energy

"   "

{ Variational. Quantum MC will

Never reach the true ground State }

$\Psi_T(\{\theta\}, \vec{R})$

A typical form for $\Psi_T(\{\theta\}, \bar{R})$

for an Intracting System reads as

Jastrow Correlation factor

$$\Psi_T(\{\theta\},\vec{R}) = \underbrace{\phi(\{\theta\},\vec{R})}_{\text{for Non-Interacting System}}\, e^{-U(R)}$$

Interaction with External field

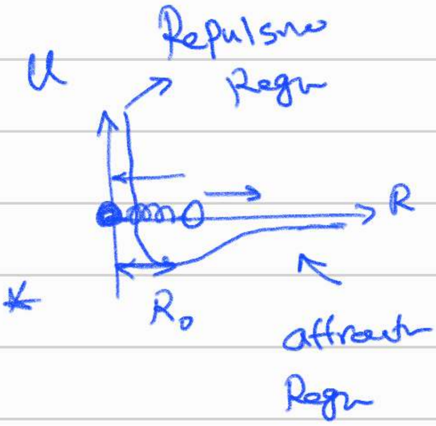
$$U(\vec{R}) = \sum_{i=1}^{N} u_1(\bar{R}_i) + \sum_{i,j}{}' u_2(R_i,R_j) + \sum_{ijk} u_3(R_i,R_j,R_k)$$

$$\underbrace{u_2(\bar{R}_i,\bar{R}_j)} = \frac{\theta_1}{R^{12}} - \frac{\theta_2}{R^{6}} \qquad R = |R_i - R_j|$$

typical Semi-empirical formula

(Lennard-Jonse 1924)

$$u(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]. \;*$$



$\{\epsilon,\sigma\} \rightarrow$ it can be determined via Experiment

$$H = \sum_{i=1}^{N} H_i \Rightarrow E_L = \sum_{i=1}^{N} E_L^{(i)} = \sum \frac{H_i \Psi_T}{\Psi_T}$$

N=2

$$\mathcal{H}_i = \frac{\partial^2}{\partial x_i^2}$$

$$\Psi_T = \underbrace{\Psi_1 \Psi_2} = e^{-\theta_1 x_1} e^{-\theta_2 x_2}$$

$$\frac{\mathcal{H}_1 \Psi_T}{\Psi_T} = \frac{\cancel{e^{-\theta_2 x_2}} \frac{d^2}{dx^2} e^{-\theta_1 x_1}}{e^{-\theta_1 x_1 \cancel{-\theta_2 x_2}}}$$

$$= E_L^{(1)}$$

$$E_L^{(2)}$$

تمرین

$$E_L^{(N)} = E_L^{(1)} + E_L^{(2)} + \cdots$$

Ex: $N=1$, , $D=1$

Simple Harmonic oscillator $\leftarrow$ $$\mathcal{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$$

$$\Psi_T(\theta, x) = e^{-\theta x^2}$$

$$E(\theta) = \frac{1}{N} \sum_{i=1}^{N} E_L(\theta, x_i)$$

$$p(\theta, x_i) = \frac{|\psi_T(\theta, x_i)|^2}{\int dx\, |\psi_T(\theta, x)|^2}$$

Subrotin (A)

loop $\theta = \theta_{min}, \theta_{max}, \Delta\theta$

آنقدر حالت تولید شود

Loop $i=1, N$

Subrotin (B) ← Select x_i from $P(\theta, x_i)$

$E(\theta) = E(\theta) + E_L(\theta, x_i)$

End loop

$E(\theta) = \frac{E(\theta)}{N}$

Write θ, $E(\theta)$

End loop

Assume that your Quan has e.g. 3-free Parameter $\{\theta\} : \{\theta_1, \theta_2, \theta_3\}$

فرض کنید. $\psi_T = e^{-(\theta_1 x^{\theta_2} + \theta_3)}$

MCMC

$E = 0$

$\{\theta\}_{old} = \checkmark$, $E_{old} = \checkmark$

loop $j = 1, \quad M$

A

$$\{\theta\}_{old} \longrightarrow \{\theta\}_{New} = \{\, \theta_1^{old} + \Delta\theta_1 ,\ \theta_2^{old} + \Delta\theta_2 ,\ \theta_3^{old} + \Delta\theta_3 ,\ \}$$

تنظیم کنیم

$$\Delta\theta_1 = a_1 \mathcal{N}(0, \sigma_1)$$

$$\Delta\theta_2 = a_2 \mathcal{N}(0, \sigma_2)$$

$$\Delta\theta_3 = a_3 \mathcal{N}(0, \sigma_3)$$

Gaussian funct

$x_{old} = \checkmark$

Loop $j = 1 \quad N$

$$E(j) = E(j) + E_L(\{\theta\}_{New}, x_{old})$$

$$P(x_{old}) = |\psi_T(\{\theta\}_{New}, x_{old})|^2$$

$$x_{old} \longrightarrow x_{New} = x_{old} + \Delta x$$

$$\boxed{\Delta x = a_4 \mathcal{N}(0, \sigma_4)}$$

$$P(x_{New}) = \checkmark$$

اینقدر تا مطمئن هستیم که x های تولید شده دارای تابع توزیع $P(x|\{\theta\})$ هستند

$$AR = \min\left\{1, \frac{P(x_{New})}{P(x_{old})}\right\}$$

B

Metropolis

End loop

$$E(j) = \frac{E(i)}{N}$$

A

$$E_{New} = E(j)$$

$$AR = \min\left\{1, \frac{E_{old}}{E_{New}}\right\}.$$

Metropolis

y = Call Random Number

if $y \leq \frac{E_{old}}{E_{New}}$

$E_{old} = E_{New}$

$\{\theta\}_{old} = \{\theta\}_{New}$

End if

End loop.