Sheet ______ Date

$$\sum_i \left(-\frac{\hbar^2}{2m}\nabla_i^2\right) + \sum_\alpha \sum_i \left(\frac{g_\alpha(-)e}{4\pi\varepsilon_0 |R_\alpha - r_i|}\right) + \sum_i \sum_j \left[\frac{e^2}{4\pi\varepsilon_0 |r_i - r_j|}\right] + \sum_\alpha \sum_\beta \left[\frac{g_\alpha g_\beta}{4\pi\varepsilon_0 |R_\alpha - R_\beta|}\right]$$

$$E = \langle \phi(x_1 \cdots x_N) | H | \phi(x_1 \cdots x_N) \rangle \rightarrow \frac{\partial E}{\partial \phi} \Rightarrow h = -\frac{\hbar^2}{2m}\nabla^2 + \sum_\alpha \frac{g_\alpha(-e)}{4\pi\varepsilon_0 |R_\alpha - r|} + \sum_j \int \frac{\phi_j^*(r_j)\phi(r_j)\times}{4\pi\varepsilon_0 |r_j - r|}$$

$$\frac{1}{\sqrt{N_i}} \begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_N(x_1) \\ \vdots & & & \\ \phi_N(x_N) & \phi_N(x_N) & \cdots & \phi_N(x_N) \end{pmatrix}$$

$$h\phi(r) = \varepsilon_i \phi_i(r).$$

$$\rightarrow \sum_\mu^K c_\mu b_\mu(r) \Rightarrow \begin{pmatrix} \langle b_1|h|b_1\rangle & \cdots & \langle b_K|h|b_1\rangle \\ \langle b_K|h|b_K\rangle & \cdots & \langle b_K|h|b_K\rangle \end{pmatrix} \times \begin{pmatrix} c_1 \\ \vdots \\ c_K \end{pmatrix} = \varepsilon_i \begin{pmatrix} \langle b_1|b_1\rangle & \cdots \\ \langle b_K|b_1\rangle & \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_K \end{pmatrix}$$

미분해서 얻은

Many body | Single body.

virtual
occupied.
HF=N개의 solution.

(벡터 함수 가능해)
energy band gap
가능
overlap 아닐때
but exchange해
보기능

$$\text{"} = K \; N$$

$$c_0\phi(x_1 \cdots x_N) + c_1\phi'(x_1 \cdots x_N) \quad c_0 = 2. \quad c_1 = 0.$$

linear combination
E가 더 ...
⇓
configuration

$$\phi = \sum c_\mu^{(i)} b_\mu(r).$$

하트리fock으로 얻어서 N개
지정은 . 얻어서 N+H 되어 해에 linear 조합 적용.
(virtual orbital 만드는 것은 base set 만드는 것과 같은
관계로 계수 C 구하기)
HF ⇒ base set 찾는 것 of many body

HF 관점에서 보면

$$\psi = \sum_K d_K \phi_\phi^{(K)}(x_1 \cdots x_N).$$

이런 세팅 이미

$$H\psi = E\psi.$$

$$H \left| \sum_\ell d_\ell \phi^\ell(x_1 \cdots x_N) \right\rangle = E \left| \sum_\ell d_K \phi^\ell(x_1 \cdots x_N) \right\rangle.$$

K=60, N

$$4C_1C$$

$$\psi(0)(i)\; NC_1(2K-\tfrac{N}{2})C_1$$

1개 취할 방식.

$$\rightarrow \phi_1^K \; ; \text{그런} \downarrow$$

(ii) 2개 excite될 방식. ⇒

$$NC_2(2K-\tfrac{N}{2})C_2$$

⇓
불가능 pauli 배타원리에 의해.

$$\frac{1}{\sqrt{N}} \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_N(x_1) \\ \phi_N(x_N) & \cdots & \phi_N(x_N) \end{pmatrix}.$$

"

$$\begin{pmatrix} \langle\phi^1|H|\phi^1\rangle & \langle\phi^2|H|\phi^2\rangle & \cdots & \langle\phi^\ell|H|\phi^\ell\rangle \\ \vdots & & & \\ \langle\phi^\ell|H|\phi^\ell\rangle & \cdots & & \langle\phi^\ell|H|\phi^\ell\rangle \end{pmatrix} \times \begin{pmatrix} d_1 \\ \vdots \\ d_\ell \end{pmatrix}$$

antisymmetry many body.

"

$$\int \frac{\det}{\sqrt{N_i}} \begin{pmatrix} \phi_1^*(x_1) & \phi_N^*(x) \\ \phi_1^*(x_N) & \cdots \phi_N(x_N) \end{pmatrix} \frac{\det}{\sqrt{N_i}} \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_N(x_1) \\ \phi_1(x_N) & \cdots & \phi_N(x_N) \end{pmatrix} E \; d(x_1 dx_2 \cdots dx_N).$$

$$\begin{pmatrix} \langle\phi^1|\phi^1\rangle & \langle\phi^1|\phi^2\rangle & \cdots & \langle\phi^1|\phi^\ell\rangle \\ & \langle\phi^\ell|\phi^\ell\rangle & & \\ \langle\phi^\ell|\phi^\ell\rangle & & \cdots & \end{pmatrix} \begin{pmatrix} d_1 \\ \vdots \\ d_\ell \end{pmatrix}$$

ϕ_2
ϕ_1
ϕ_1

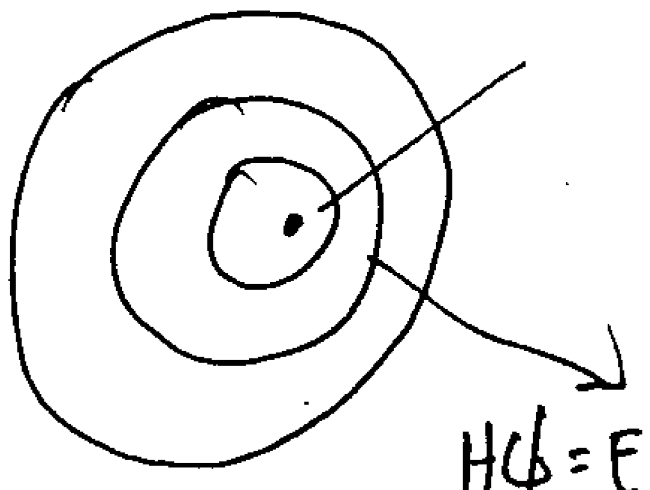
$\psi_0 = \frac{\det}{\sqrt{2}} \begin{pmatrix} \phi_1(x_1) & \phi_1(x_1) \\ \phi_1(x_2) & \phi_1(x_2) \end{pmatrix}$

3th $\psi_1 = \frac{\det}{\sqrt{2}} \begin{pmatrix} \phi_1(x_1) & \phi_3(x_2) \\ \phi_1(x_2) & \phi_3(x_2) \end{pmatrix}$

7th $\psi_2 = \frac{\det}{\sqrt{2}} \begin{pmatrix} \phi_1(x_1) & \phi_7(x_1) \\ \phi_1(x_2) & \phi_7(x_2) \end{pmatrix}$

5-7 $\vdots$ $(\phi_5\ \phi_7)$ 이런식. $\longrightarrow$ infinite L 또 CI ? full

이론만 있는 가상적.



system 전체 E에서 antisymmetry때

$H\psi = E\psi \Rightarrow E = \langle\psi|H|\psi\rangle \Rightarrow \boxed{\frac{\partial E}{\partial \phi_i^*} \quad \int \rho\, dr = N} \Rightarrow h\phi_i = \epsilon\phi_i$

? $\sum \phi_i^*(x)\phi_i(x)$?

또 $\sum^{k} d_k b_k(k)$

직접적으로 풀기 힘들때 mathematical 가능.

so 여기에 대입

이용

없음.

$K>N$ solution

ground state 구하게 됨

↑ 이러한 basis set 가지고는 안됨 many body 위한 base set 만들.

$L:\infty$ full CI
(Configuration Interation)

$$\rho(r) = \sum_{\alpha=1}^{N} \underline{\phi_a^*(r)\,\phi_a(r)}$$
Norm. 크기.

$$\int \rho(r)\,dr = \sum_{\alpha=1}^{N} \underbrace{\int \phi_a^*(r)\phi_a(r)\,dr}_{1}$$
$$= \sum_{\alpha=1}^{N} 1 = N.$$