09.08 2nd.

Review 1 dimension.

$$f(x.t)=\frac{1}{\sqrt{2\pi\hbar}}\int C_0 \exp\left(\frac{i}{\hbar}(px-\omega t)\right)dp$$

$$C_p=\frac{1}{\sqrt{2\pi\hbar}}\int f(x.t)\exp\left(-\frac{i}{\hbar}\cdot px\right)dx.$$

3 dim $\Downarrow$

$$f(r.t)=\frac{1}{\sqrt{2\pi\hbar}^3}\iiint C_p \exp\left(\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-\omega t)\right)d^3p$$

$$C_p=\left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3\int f(r.t)\exp -\frac{i}{\hbar}(p\vec{r})\,d^3r.$$

$$p=\hbar \overset{\frac{2\pi}{\lambda}}{K},\quad E=\overset{\frac{2\pi}{T}}{\omega}\hbar \text{ 58}$$

1 dim

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]f(x.t)=Ef(x.t)$$

$\Downarrow$

$$\dashrightarrow \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\frac{1}{h_1h_2h_3}\Sigma\frac{\partial}{\partial x_j}\frac{h_1h_2h_3}{h_j^2}\frac{\partial}{\partial x_j}$$

3dim

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]f(r.t)=Ef(r.t).$$

Laplacian $\Rightarrow$

$$\dashrightarrow \frac{1}{r^2\sin\theta}\left[\frac{\partial}{\partial r}\left(\frac{r^2\sin\theta}{1}\right)\frac{\partial}{\partial r}+\frac{\partial}{\partial\theta}\left(\frac{r^2\sin\theta}{r^2}\right)\frac{\partial}{\partial\theta}+\frac{\partial}{\partial\phi}\frac{r^2\sin\theta}{(r\sin\theta)^2}\frac{\partial}{\partial\phi}\right]$$

* Coordination

Cartesian : $h_1=h_2=h_3=1$

$x_1=x,\ x_2=y,\ x_3=z$

cylinder : $h_1=1\quad h_2=r\quad h_3=1$

$x_1=r\quad x_2=\theta\quad x_3=z$

spherical : $h_1=1\quad h_2=r\quad h_3=r\sin\theta.$

$x_1=r\quad x_2=\theta\quad x_3=\phi$

Pauli exclusive

e^- —— $Q_a(r)\beta$

e^- —— $Q_a(r)\alpha$

$$\frac{1}{\sqrt{2i}}\begin{pmatrix}\phi_a(r_1)\beta(1) & \phi_a(r_1)\beta(1)\\ \phi_a(r_2)\beta(2) & \phi_a(r_2)\beta(2)\end{pmatrix} = 0$$

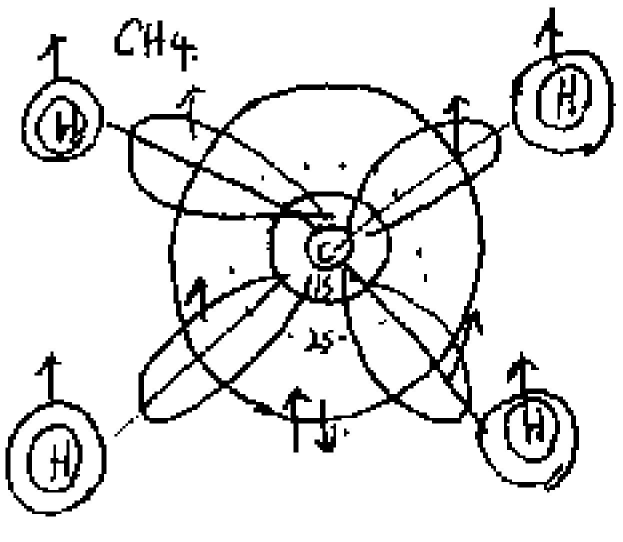
$$\frac{1}{\sqrt{2!}}\begin{pmatrix}\phi_a(r_1)\alpha(1) & \phi_a(r_1)\beta(1)\\ \phi_a(r_2)\alpha(2) & \phi_a(r_2)\beta(2)\end{pmatrix} \neq 0$$

$$\sum_{\alpha} -\frac{\hbar^2}{2m_\alpha}\nabla_\alpha + \sum_{K} -\frac{\hbar^2}{2M_K}\nabla_K$$

$$+ \sum_{\alpha}\sum_{K}\frac{q_a(-e)}{4\pi\varepsilon_0|R_a-R_K|} + \sum_{\alpha}\sum_{\beta>\alpha}\frac{q_\alpha q_\beta}{4\pi\varepsilon_0|R_\alpha-R_\beta|} + \sum_{K}\sum_{l>K}\frac{(-e)^2}{4\pi\varepsilon_0|\quad -r_l|}$$

$$\hat{H}\quad\frac{1}{\sqrt{N_!}}\det\begin{vmatrix}\phi_a(1)\phi_b(1)\cdots\\ \phi_a(2)\phi_b(2)\cdots\\ \\ \phi_a(N)\phi_b(N)\cdots\end{vmatrix} = E\left(\frac{1}{\sqrt{N_!}}\right)\det\begin{vmatrix}\overbrace{\phi_a(1)\ \phi_b(1)\ \cdots}^{N}\\ \phi_a(2)\quad\cdots\\ \\ \phi_a(N)\quad\cdots\end{vmatrix}$$

$f(x_1 x_2 \cdots ;t)$



핵의 K.E

$$\sum_{\alpha=1}^{5} -\frac{\hbar^2}{2M_\alpha}\cdot\nabla_\alpha^2 = -\frac{\hbar^2}{2m_c}\nabla_c^2 - \frac{\hbar^2}{2m}\nabla_{H1}^2 - \frac{\hbar^2}{2m}\nabla_{H2}^2 - \frac{\hbar^2}{2m}\nabla_{H3}^2 - \frac{\hbar^2}{2m}\nabla_{H4}^2$$

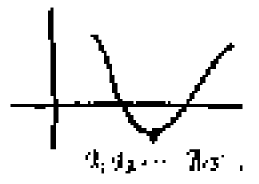
electron (10개) K.E.

$$\sum_{k=1}^{10}\left(-\frac{\hbar^2}{2m_e}\nabla_{ek}^2\right)$$

$f(x_1 \cdots x_{15}, t)$
$= E f(x_1 \cdots x_{15}, t)$ ←

interaction (P.E)

$$+\sum_{\alpha}^{5}\sum_{k}^{10}\frac{g_\alpha(-e)}{4\pi\epsilon_0|R_\alpha - r_k|} + \sum_{\substack{\alpha,\beta\\ \beta>\alpha}}\frac{g_\alpha g_\beta}{4\pi\epsilon_0|R_\alpha R_\beta|} + \sum_{\substack{k,l\\ l>k}}\frac{(e)(-e)}{4\pi\epsilon_0|r_l r_k|}$$



Reality $E = mc^2$

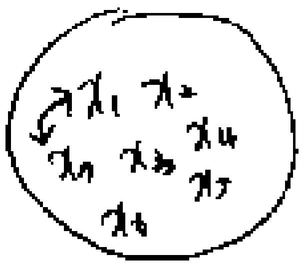
$$\downarrow$$

$$\frac{m_0}{\sqrt{1-\left(\frac{v}{c}\right)^2}}c^2 , \quad f(x) = \sum\frac{f^K(0)}{K!}(x-0)^k$$

$$= m_0c^2\left(1+\frac{1}{2}\left(\frac{v}{c}\right)^2 + \frac{1}{2}\left(\frac{3}{4}\right)\left(\frac{v}{c}\right)^4 + \cdots\right) = m_0c^2 + \frac{1}{2}m_0v^2 + \frac{3}{8}m_0\left(\frac{v^4}{c^2}\right) + \cdots$$

(정지시 원래 물체 갖는 E = 운동 E) $\rightarrow m_0c^2 = \frac{1}{2}m_0v^2 + \cdots\cdots$

$$\therefore E = \frac{p^2}{2m} + \underbrace{\frac{3}{8}\frac{p^4}{m^3c^2}}_{\text{상대적 개념 포함}} + V(x.y.t)$$

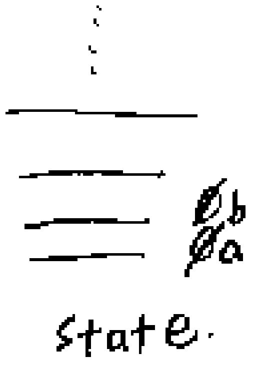


$$f^2(x_1 x_2 \cdots x_n, t) = f^2(x_n \cdots x_1, t)$$

$$a^2 = b^2 \begin{cases} a = b & \text{Boson} \\ a = -b & \text{Fermion.} \end{cases}$$

$$\det\begin{vmatrix} X_a(1) & X_b(1) \\ X_a(2) & X_b(2) \end{vmatrix} = \underline{X_a(1)X_b(2) - X_b(1)X_a(2) = A}$$

전자 위치 바꾸면 $\underline{-A}$가 됨.



$$\frac{1}{\sqrt{N!}}\det\begin{vmatrix} \overbrace{\phi_a(1)\ \phi_b(1) \cdots \phi_?(1)}^{N} \\ \phi_a(2)\ \phi_b(2) \cdots \phi_?(2) \\ \\ \phi_a(N)\ \phi_b(N) \cdots \phi_?(N) \end{vmatrix} = f(x_1 \cdots x_4)$$

$$\text{ex)}\ f(x_1, x_2) = \frac{1}{\sqrt{2!}}\det\begin{vmatrix} \phi_a(1) & \phi_b(1) \\ \phi_a(2) & \phi_b(2) \end{vmatrix} = \frac{1}{\sqrt{2}}\left(\phi_a(1)\phi_b(2) - \phi_b(1)\phi_a(2\right.$$