©2022 YHAL, YITP, Kyoto University
京都大学基礎物理学研究所　湯川記念館史料室

N18

野間氏の計算 II.

1.

$\overline{\overline{\sigma}}(x)$.　　$\sigma(x) = -e\hat{\psi}\psi$.

$$\psi = \sum_{\alpha,i} a_{\alpha i} u_{\alpha i} + \sum_i b_i v_i$$

$u_{\alpha i}(\vec{r}) = u_i(\vec{r} - \vec{R}_\alpha)$ は $\vec{R}_\alpha$ にある原子に束縛された電子の i-state の波動函数.

$$\hat{\psi} = \sum_{\alpha,i} a^*_{\alpha i} \tilde{u}_{\alpha i} + \sum_i b_i^* \tilde{v}_i$$

$$a^*_{\alpha i} a_{\beta j} + a_{\beta j} a^*_{\alpha i} = \delta_{\alpha,\beta}\delta_{ij}.$$

$v_i(\vec{r})$ 自由電子の波動函数.

$$\left.\begin{aligned} &a^*_{\alpha i} a_{\alpha i} = n_{\alpha i} \qquad \sum_i n_{\alpha i} = n_\alpha \\ &\Theta = \int e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv' = (\sqrt{\pi} a)^3. \end{aligned}\right\}$$ とする。

$$\overline{\overline{\sigma}}(\vec{x}) = \frac{1}{\Theta}\int \sigma(\vec{x}') e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv'$$

$$\begin{aligned} = -\frac{e}{\Theta}\Bigg[&\sum_{\alpha i} a^*_{\alpha i} a_{\alpha i} \int \tilde{u}_i(\vec{r}'-\vec{R}_\alpha) u_i(\vec{r}'-\vec{R}_\alpha) e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv' \\ &+ \sum_i b_i^* b_i \int \tilde{v}_i(\vec{r}') v_i(\vec{r}') e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv' \\ &+ \sum_{\alpha\neq\beta, ij} a^*_{\alpha i} a_{\beta j} \int \tilde{u}_i(\vec{r}'-\vec{R}_\alpha) u_j(\vec{r}'-\vec{R}_\beta) e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv' \\ &+ \sum_{\alpha ij} a^*_{\alpha i} b_j \int \tilde{u}_i(\vec{r}'-\vec{R}_\alpha) v_j(\vec{r}') e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv' \\ &+ \sum_{\alpha ij} b_j^* a_{\alpha i} \int u_i(\vec{r}'-\vec{R}_\alpha) \tilde{v}_j(\vec{r}') e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}} dv' \Bigg] \end{aligned} \qquad (1)$$

N19 050

c031-030-050

©2022 YHAL, YITP, Kyoto University
京都大学基礎物理学研究所　湯川記念館史料室

(1) の第一項.

$$-\frac{e}{\Theta}\sum_{\alpha i} a^*_{\alpha i} a_{\alpha i}\int \tilde{u}_i(\vec r'-\vec R_\alpha)\, u_i(\vec r'-\vec R_\alpha)\, e^{-\frac{|\vec r'-\vec r|^2}{a^2}}\, dv'$$

$$= -\frac{e}{\Theta}\sum_{\alpha i} n_{\alpha i}\int |u_i(\vec r'-\vec R_\alpha)|^2\, e^{-\frac{|(\vec R_\alpha-\vec r)+(\vec r'-\vec R_\alpha)|^2}{a^2}}\, dv'$$

$$\simeq -\frac{e}{\Theta}\sum_{\alpha i} n_{\alpha i}\int |u_i(\vec r'-\vec R_\alpha)|^2 \left\{ e^{-\frac{|\vec R_\alpha-\vec r|^2}{a^2}} + (\vec r'-\vec R_\alpha)\cdot\mathrm{grad}_\alpha\, e^{-\frac{|\vec R_\alpha-\vec r|^2}{a^2}} \right\} dv'$$

$$= -\frac{e}{\Theta}\sum_{\alpha i} n_{\alpha i}\, e^{-\frac{|\vec R_\alpha-\vec r|^2}{a^2}} - \frac{e}{\Theta}\left(\sum_{\alpha i} n_{\alpha i}\int (\vec r'-\vec R_\alpha)\,|u_i(\vec r'-\vec R_\alpha)|^2\, dv'\right)\cdot\mathrm{grad}_\alpha\, e^{-\frac{|\vec R_\alpha-\vec r|^2}{a^2}}.$$

$$= -\frac{e}{\Theta}\sum_{\alpha} n_\alpha\, e^{-\frac{|\vec R_\alpha-\vec r|^2}{a^2}} + \frac{1}{\Theta}\sum_{\alpha} \vec p_\alpha\cdot\mathrm{grad}_\alpha\, e^{-\frac{|\vec R_\alpha-\vec r|^2}{a^2}}.$$

ここに.

$$\vec p_\alpha = \sum_i -e\, n_{\alpha i}\int |u_i(\vec r'-\vec R_\alpha)|^2\cdot(\vec r'-\vec R_\alpha)\, dv' \qquad (2).$$

は $\vec R_\alpha$ にある原子の電気能率.

更に

$N(\vec r)$ を原子の number density とすれば $\sum_\alpha$ を積分になおして. 且 index α を落して. $n_\alpha = n(R)$ 等と書けば 上式は

$$= -\frac{e}{\Theta}\int N(\vec R)\, n(\vec R)\, e^{-\frac{|\vec R-\vec r|^2}{a^2}}\, dV + \frac{1}{\Theta}\int N(R)\,\vec p(R)\,\mathrm{grad}_R\, e^{-\frac{|\vec R-\vec r|^2}{a^2}}\, dV.$$

$$= -e\, N(\vec r)\,\bar{\bar n}(\vec r) - \frac{1}{\Theta}\int \left(\mathrm{div}_R\, N(\vec R)\,\vec p(\vec R)\right) e^{-\frac{|\vec R-\vec r|^2}{a^2}}\, dV.$$

$$= -e\, N(\vec r)\,\bar{\bar n}(\vec r) - \frac{1}{\Theta}\,\mathrm{div}\left\{ N(\vec r)\int \vec p(\vec R)\, e^{-\frac{|\vec R-\vec r|^2}{a^2}}\, dV \right\}.$$

$$= N(\vec r)\left\{-e\,\bar{\bar n}(r)\right\} - \mathrm{div}\left\{N(\vec r)\,\bar{\bar{\vec p}}(\vec r)\right\}.$$

$$\left.\begin{aligned} \bar{\bar{\vec p}}(\vec r) &= \frac{1}{\Theta}\int \vec p(\vec R)\, e^{-\frac{|\vec R-\vec r|^2}{a^2}}\, dV. \\ \bar{\bar n}(r) &= \frac{1}{\Theta}\int n(\vec R)\, e^{-\frac{|\vec R-\vec r|^2}{a^2}}\, dV \end{aligned}\right\} \quad (3)$$

は r にある一つの原子に束縛された電子の平均の数

©2022 YHAL, YITP, Kyoto University
京都大学基礎物理学研究所　湯川記念館史料室

(1)の第二項

$$-\frac{e}{\textcircled{H}}\sum_i n_i \int |v_i(r')|^2 e^{-\frac{|\vec{x}'-\vec{x}|^2}{a^2}}\,dv'$$

$$= -\,e N_c(\vec{x}). \qquad N_c(\vec{x}) = \frac{1}{\textcircled{H}}\sum_i n_i \int \overbrace{|v_i(\vec{r}')|^2}^{=1} e^{-\frac{|\vec{x}'-\vec{x}|^2}{a^2}}\,dv' \quad (4)$$

$=\sum_i n_i$ は自由電子の number density.

故に核（原子番号Z）の contribution をも考慮すれば ~~(1). (2). (3) より~~

$$\bar{\bar{\sigma}}(\vec{x}) = N(\vec{x})\, e\{Z - \bar{\bar{n}}(\vec{x})\} - eN_c(\vec{x}) - \mathrm{div}\, N(\vec{x})\,\bar{\bar{\vec{p}}}(\vec{x}) + \cdots\cdots$$

$$= \rho(\vec{x}) - \mathrm{div}\,\vec{P}(\vec{x}) + \cdots\cdots \qquad \cancel{(4)}\ (5)$$

但し

$$\left.\begin{aligned} \rho(\vec{x}) &= N(\vec{x})\, e\{Z - \bar{\bar{n}}(\vec{x})\} - eN_c(\vec{x}). \\ \vec{P}(\vec{x}) &= N(\vec{x})\,\bar{\bar{\vec{p}}}(\vec{x}) \end{aligned}\right\} \quad (6).$$