野崎氏の計算、

$$\left[\ \overline{\overline{\vec{j}}}(\vec{r})\ \right].$$

$$\tilde{\psi} = \sum_k a_k^* \tilde{u}_k \qquad \psi = \sum_k a_k u_k$$

$u_k = u_i(\vec{r} - \vec{R}_\alpha)$ ：$\vec{R}_\alpha$にある原子に束縛されてゐる場合.
$u_k = v_i(\vec{r})$. 自由なる場合. (1)

$$\vec{j} = -\frac{e\hbar}{2im}(\tilde{\psi}\,\mathrm{grad}\,\psi - \mathrm{grad}\,\tilde{\psi}\cdot\psi) - \frac{e^2}{mc}\tilde{\psi}\psi\vec{A}.$$
$$= -\frac{e\hbar}{2im}\sum_{kl} a_k^* a_l(\tilde{u}_k\,\mathrm{grad}\,u_l - \mathrm{grad}\,\tilde{u}_k\cdot u_l) - \frac{e^2}{mc}\sum_{kl} a_k^* a_l \tilde{u}_k u_l \vec{A}$$
$$= \sum_{kl}\vec{j}_{kl}.$$
$$\vec{j}_{kl} = -\frac{e\hbar}{2im} a_k^* a_l(\tilde{u}_k\,\mathrm{grad}\,u_l - \mathrm{grad}\,\tilde{u}_k\cdot u_l) - \frac{e^2}{mc} a_k^* a_l \tilde{u}_k u_l \vec{A}. \qquad (2)$$

$$\sigma = -e\tilde{\psi}\psi$$
$$= -e\sum_{k,l} a_k^* a_l \tilde{u}_k u_l.$$
$$= \sum_{k,l}\sigma_{kl}.$$
$$\sigma_{kl} = -e\,a_k^* a_l \tilde{u}_k u_l. \qquad (3)$$

$$\mathrm{div}\,\vec{j} + \frac{\partial\sigma}{\partial t} = 0$$
$$\mathrm{div}\,\vec{j}_{kl} + \frac{\partial\sigma_{kl}}{\partial t} = 0. \qquad (4).$$

$$\overline{\overline{\vec{j}}}(\vec{r}) = \frac{1}{\textcircled{H}}\sum_k \int \vec{j}_{kk}(\vec{r}')\,e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}dv' + \frac{1}{\textcircled{H}}\sum_{k\neq l}\int \vec{j}_{kl}(\vec{r}')\,e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}dv' \qquad (5).$$

次に (5) の第一項を計算。

N19 060

c031-030-060

$U_k(\vec{r}') = v_i(\vec{r}')$ なる部分をとれば

$$\frac{1}{H}\sum_k \int \vec{j}_{kk}(\vec{r}')\, e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}\, dv'$$

$$= -\frac{e}{H}\sum_i a_i^* a_i \int \Big[\frac{\hbar}{2im}\Big\{\tilde{v}_i(\vec{r}')\,\mathrm{grad}_{r'} v_i(\vec{r}') - \mathrm{grad}_{r'}\tilde{v}_i(\vec{r}')\cdot v_i(\vec{r}')\Big\} + \frac{e}{mc}\tilde{v}_i(\vec{r}')\, v_i(\vec{r}')\,\vec{A}(\vec{r}')\Big] \times e^{-\frac{|r'-r|^2}{a^2}}\, dv'$$

$$= -e\sum_i \frac{n_i}{H}\int \tilde{v}_i(\vec{r}')\Big\{\frac{\hbar}{im}\,\mathrm{grad}_{r'} + \frac{e}{mc}\vec{A}(\vec{r}')\Big\} v_i(\vec{r}')\, e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}\, dv'$$

$$- \frac{e\hbar}{2im}\sum_i \frac{n_i}{H}\int \tilde{v}_i(\vec{r}')\, v_i(\vec{r}')\,\mathrm{grad}_{r'}\, e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}\, dv'$$

$$= \vec{j}_c(\vec{r}) + \frac{e\hbar}{2im}\,\mathrm{grad}_r\, N_c(\vec{r}). \qquad (6)$$

但し

$$\left.\begin{aligned} \vec{j}_c(\vec{r}) &= -e\sum_i \frac{n_i}{H}\int \tilde{v}_i(\vec{r}')\Big\{\frac{\hbar}{im}\,\mathrm{grad}_{r'} + \frac{e}{mc}\vec{A}(\vec{r}')\Big\} v_i(\vec{r}')\, e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}\, dv'. \\ N_c(\vec{r}) &= \sum_i \frac{n_i}{H}\int \tilde{v}_i(\vec{r}')\, v_i(\vec{r}')\, e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}\, dv' \end{aligned}\right\} \quad (7).$$

$u_k(\vec{r}') = u_i(\vec{r}'-\vec{R}_\alpha)$ なる部分をとり，この場合の

$\vec{j}_{kk}(\vec{r}')$, $\sigma_{kk}(\vec{r}')$ を夫々 $\left\{\begin{array}{l}\vec{j}_{\alpha i} \text{ 又は } \vec{j}_i(\vec{r}'-\vec{R}_\alpha) \\ \sigma_{\alpha i} \text{ 又は } \sigma_i(\vec{r}'-\vec{R}_\alpha)\end{array}\right\}$ と書くことにすれば

$$\frac{1}{\Theta}\sum_k \int \vec{j}_{kk}(\vec{r}')\, e^{-\frac{|\vec{r}'-\vec{r}|^2}{a^2}}\, dv'$$

$$= \frac{1}{\Theta}\sum_{\alpha i}\int \vec{j}_i(\vec{r}'-\vec{R}_\alpha)\, e^{-\frac{|(\vec{R}_\alpha-\vec{r})+(\vec{r}'-\vec{R}_\alpha)|^2}{a^2}}\, dv'$$

$$\simeq \frac{1}{\Theta}\sum_{\alpha i}\int \vec{j}_i(\vec{r}'-\vec{R}_\alpha)\left\{e^{-\frac{|\vec{R}_\alpha-\vec{r}|^2}{a^2}} + (\vec{r}'-\vec{R}_\alpha)\,\mathrm{grad}_\alpha\, e^{-\frac{|R_\alpha-r|^2}{a^2}}\right\} dv' \qquad (8).$$

$\left(\dfrac{|\vec{r}'-\vec{R}_\alpha|}{a}\right.$ の一次の項まで).

之を計算する為に次の関係を利用する。

$\left.\begin{array}{l}\vec{r}'-\vec{R}_\alpha = \vec{\xi} \\ \vec{R}_\alpha-\vec{r} = \vec{\zeta}\end{array}\right\}$ と書けば

$$\int \vec{j}_i(\vec{\xi})\, dv' = -\int \mathrm{div}_{r'}\, \vec{j}_i(\vec{\xi})\cdot \vec{\xi}\, dv' = \int \frac{\partial \sigma_{\alpha i}}{\partial t}\, \vec{\xi}\, dv'$$

$$= \frac{\partial}{\partial t}\left\{-e\, n_{\alpha i}\int \hat{u}_i(\vec{\xi})\, \vec{\xi}\, u_i(\vec{\xi})\, dv'\right\} \quad (\text{核の運動を無視})$$

$$= \frac{\partial \vec{p}_{\alpha i}}{\partial t}. \qquad (9).$$

$$\int\left\{\vec{j}_i(\vec{\xi})\left(\vec{\xi}\cdot\mathrm{grad}_\alpha e^{-\frac{|\vec\eta|^2}{a^2}}\right)+\vec{\xi}\left(\vec{j}_i(\vec{\xi})\cdot\mathrm{grad}_\alpha e^{-\frac{|\vec\eta|^2}{a^2}}\right)\right\}dv' = -\int \mathrm{div}_{r'}\vec{j}_i(\vec{\xi})\cdot\vec{\xi}\left(\vec{\xi}\cdot\mathrm{grad}_\alpha e^{-\frac{|\vec\eta|^2}{a^2}}\right)dv'$$

$$=\frac{\partial}{\partial t}\int\sigma_i(\vec{\xi})\cdot\vec{\xi}\left(\vec{\xi}\cdot\mathrm{grad}_\alpha e^{-\frac{|\vec\eta|^2}{a^2}}\right)dv'$$

$$=-2e^{-\frac{|\vec\eta|^2}{a^2}}\frac{\partial}{\partial t}\int\sigma_i(\vec{\xi})\frac{\vec{\xi}}{a}\left(\frac{\vec{\xi}}{a}\cdot\vec{\eta}\right)dv'$$

$$\simeq 0 \qquad (10)$$

（被積分函数は $\frac{|\vec\xi|}{a}$ の二次のorder）.

$$\int\left\{\quad〃\quad - \quad〃\quad\right\}dv' = -\mathrm{grad}_\alpha e^{-\frac{|\vec\eta|^2}{a^2}}\times\int\vec{\xi}\times\vec{j}_i(\vec{\xi})\,dv'$$

$$=-2c\,\mathrm{grad}_\alpha e^{-\frac{|\vec\eta|^2}{a^2}}\times\vec{m}_{\alpha i} \qquad (11)$$

但し

$$\vec{m}_{\alpha i}=\frac{-e}{2c}n_{\alpha i}\int\tilde{u}_i(\vec{r}'-\vec{R}_\alpha)\left\{\frac{\hbar}{im}\mathrm{grad}_{r'}+\frac{e}{mc}\vec{A}(\vec{r}')\right\}u_i(\vec{r}'-\vec{R}_\alpha)\,dv' \qquad (12)$$

(11)の最後の形は次になる。

$$\int\vec{\xi}\times\vec{j}_i(\vec{\xi})\,dv' = -e\,n_{\alpha i}\int\vec{\xi}\times\left\{\tilde{u}_i(\vec{\xi})\frac{\hbar}{2im}\mathrm{grad}_{r'}u_i(\vec{\xi})-\frac{\hbar}{2im}\mathrm{grad}_{r'}\tilde{u}_i(\vec{\xi})\cdot u_i(\vec{\xi})+\frac{e}{mc}\vec{A}(\vec{r}')\tilde{u}_i(\vec{\xi})u_i(\vec{\xi})\right\}dv'$$

（才二項を部分積分して）

$$=-e\,n_{\alpha i}\int\vec{\xi}\times\left\{\tilde{u}_i(\vec{\xi})\frac{\hbar}{im}\mathrm{grad}_{r'}u_i(\vec{\xi})+\frac{e}{mc}\vec{A}(\vec{r}')\tilde{u}_i(\vec{\xi})u_i(\vec{\xi})\right\}dv'$$

$$=2c\left[\frac{-e\,n_{\alpha i}}{2c}\int\tilde{u}_i(\vec{\xi})\left\{\vec{\xi}\times\left(\frac{\hbar}{im}\mathrm{grad}_{r'}+\frac{e}{mc}\vec{A}(\vec{r}')\right)\right\}u_i(\vec{\xi})\,dv'\right.$$

(10) + (11) より.

$$\int\vec{j}(\vec{r}'-\vec{R}_\alpha)\left((\vec{r}'-\vec{R}_\alpha)\cdot\mathrm{grad}_\alpha e^{-\frac{|\vec{R}_\alpha-\vec{r}'|^2}{a^2}}\right)dv' = -c\,\mathrm{grad}_\alpha e^{-\frac{|\vec{R}_\alpha-\vec{r}'|^2}{a^2}}\times\vec{m}_{\alpha i} \qquad (13)$$

(9) 及び (13) を (8) に代入すれば

$$(8) = \frac{1}{H}\sum_{\alpha i}\frac{\partial \vec{p}_{\alpha i}}{\partial t} e^{-\frac{|\vec{R}_\alpha-\vec{r}|^2}{a^2}} - \frac{c}{H}\sum_{\alpha i}\mathrm{grad}_\alpha\, e^{-\frac{|\vec{R}_\alpha-\vec{r}|^2}{a^2}} \times \vec{m}_{\alpha i}$$

$$= \frac{1}{H}\sum_{\alpha}\frac{\partial \vec{p}_{\alpha}}{\partial t} e^{-\frac{|\vec{R}_\alpha-\vec{r}|^2}{a^2}} - \frac{c}{H}\sum_{\alpha}\mathrm{grad}_\alpha\, e^{-\frac{|\vec{R}_\alpha-\vec{r}|^2}{a^2}} \times \vec{m}_{\alpha}$$

$$\left\{ \vec{p}_\alpha = \sum_i \vec{p}_{\alpha i} \qquad \vec{m}_\alpha = \sum_i \vec{m}_{\alpha i} \right\}.$$

$$= \frac{1}{H}\int \frac{\partial \vec{p}(\vec{R})}{\partial t} N(\vec{R})\, e^{-\frac{|\vec{R}-\vec{r}|^2}{a^2}} dv - \frac{c}{H}\int \mathrm{grad}_R\, e^{-\frac{|\vec{R}-\vec{r}|^2}{a^2}} \times N(\vec{R})\,\vec{m}(\vec{R})\, dv$$

$$= \frac{\partial}{\partial t}\left\{\frac{1}{H}\int N(\vec{R})\,\vec{p}(\vec{R})\, e^{-\frac{|\vec{R}-\vec{r}|^2}{a^2}} dv\right\} + \frac{c}{H}\int \mathrm{curl}\left\{N(\vec{R})\,\vec{m}(\vec{R})\right\} e^{-\frac{|\vec{R}-\vec{r}|^2}{a^2}} dv$$

$$= \frac{\partial}{\partial t}\left\{\frac{N(\vec{r})}{H}\int \vec{p}(\vec{R})\, e^{-\frac{|\vec{R}-\vec{r}|^2}{a^2}} dv\right\} + c\,\mathrm{curl}\left\{\frac{1}{H}\int N(\vec{R})\,\vec{m}(\vec{R})\, e^{-\frac{|\vec{R}-\vec{r}|^2}{a^2}} dv\right\}$$

$$= \frac{\partial}{\partial t}\left\{N(\vec{r})\,\overline{\overline{\vec{p}}}(\vec{r})\right\} + c\,\mathrm{curl}\left\{N(\vec{r})\,\overline{\overline{\vec{m}}}(\vec{r})\right\}$$

$$= \frac{\partial \vec{P}(\vec{r})}{\partial t} + c\,\mathrm{curl}\,\vec{M}(\vec{r}). \qquad (14).$$

但し

$$\vec{P}(\vec{r}) = N(\vec{r})\,\overline{\overline{\vec{p}}}(\vec{r}), \quad \vec{M}(\vec{r}) = N(\vec{r})\,\overline{\overline{\vec{m}}}(\vec{r}) \qquad (15).$$

(5), (6), (14) より

$$\overline{\overline{\vec{j}}}(\vec{r}) = \vec{j}_c(\vec{r}) + \frac{\partial \vec{P}(\vec{r})}{\partial t} + c\,\mathrm{curl}\,\vec{M}(\vec{r}) + \frac{e\hbar}{2im}\mathrm{grad}_r N_c(\vec{r}) + \cdots \qquad (16).$$