Sheet 8

$$\Psi_{en}\{R\} = \sum_i c_{n,i} \Psi_{e,i}(\{r\}_i(\{R\}))$$

$$\Lambda_{ij} = \int d^3r \Psi^*_{e,j} \left(-\sum_I \frac{\hbar^2 \nabla^2_{\vec{R}_I}}{2M_I}\right) \Psi_{e,i} + \sum_I \frac{1}{M_I} \int d^3r \Psi^*_{e,j}(-i\hbar\nabla_{\vec{R}_I})\Psi_{e,i}(-i\hbar\nabla_{\vec{R}_I}).$$

$$\sum_j \left(\Lambda_{ij} + \delta_{ij} E_j\{R\}\right) c_{nj}\{\vec{R}\} +$$

2.1

Adiabatic theorem:

System stays in its Eigenstate if pertubation is slow and there exists a gap between the Eigenstate and other Eigenstates in the spectrum.

↳ relates to the $\Lambda_{ij}\ (i \neq j)$ terms: Wave functions mixing, allowing transitions to happen

2.2

$$\Lambda_{ii} = \int d^3r\, \Psi^*_{ei} \left(-\sum_I \frac{\hbar^2 \nabla^2_{R_I}}{2M_I}\right) \Psi_{ei} + \sum_I \frac{1}{M_I} \int d^3r\, \Psi^*_{ei}(-i\hbar \nabla_{R_I}) \Psi_{ei}(-i\hbar \nabla_{R_I})$$

$\Psi^*_{ei} = \Psi_{ei}$ & define $\frac{\hbar^2}{M_I} : a$

$$\Lambda_{ii} = \sum_I \int -\frac{a}{2} \Psi_i \nabla^2 \Psi_i\, d^3r + \overbrace{\sum_I \langle \Psi | \nabla_I | \Psi \rangle (-i\hbar \nabla_I)}^{\text{must be } 0}$$

$$\nabla \langle \Psi | \Psi \rangle = \langle \nabla \Psi | \Psi \rangle + \langle \Psi | \nabla \Psi \rangle = 0$$

let $y_i = (\nabla \Psi)_i$, $x = \Psi$

$$\langle y_i | x \rangle = -\langle x | y_i \rangle$$

$$\langle y_i | x \rangle^* = \langle x | y_i \rangle = -\langle x | y_i \rangle^* = -\langle y_i | x \rangle$$

$$\Rightarrow \langle y_i | x \rangle^* = -\langle y_i | x \rangle \Rightarrow \text{real part is } 0$$

If Ψ was real, derivative (I think) needs to be real: so $\langle \Psi | \nabla \Psi \rangle = 0$.

with that, $\Lambda_{ii} = \sum_I -\frac{\hbar^2}{2M_I} \int d^3r\, \Psi_i \nabla^2 \Psi_i$

2.3

$$\sum_j \left(\Lambda^{ij} C_{ni} + \delta_{ij} E_j(\{\vec{R}\}) C_{nj} + (V_{nn}(\{R\}) + T_n\right) C_{ni}(\{R\}) = E_n C_{ni}(\{R\})$$

i : electron
n : gesamt

$\Rightarrow i \neq j$: $(V_{nn}(\{R\}) + T_n) C_{ni}(\{R\}) = E_n C_{ni}(\{R\})$

$i = j$: $[\Lambda^{ii} + E_i(\{R\}) + V_{nn}(\{R\}) + T_n] C_{ni}(\{R\}) = E_n C_{ni}(\{R\})$

→ coefficient only depends on itself: so the eigenstates Ψ are only characterized by C_{ni}.

2.4

If Λ^{ii} is also 0, the quantummechanical effects described in the Λ^{ij} terms are neglected. But since $\hat{T}^n$ and V_{nn} are still quantummechanical operators, the ions are still be treated as a non-classic object. But I also find it fair to say that it's classical.