8 - The atomic and interaction hamiltonians

If we consider a collection of atoms each of one is localized in a different region of space, we need to consider that the wave-function ψ is an operator. As any operator

$$\hat{\psi}(\bar{x}) = \sum_j \hat{b}_j \varphi_j(\bar{x})$$

where b_j is an operator and $\varphi_j(\bar{x})$ is a function of space, solution of the Schröedinger equation.
The hermitian operator:

$$\hat{\psi}^+(\hat{x}) = \sum_j b_j^+ \varphi_j^*(\hat{x})$$

The difference here is that $\hat{\psi}(x)$ describes an electron (then a fermion) and it must obey Pauli's principle of exclusion. This implies:

$$\begin{cases} \hat{\psi}(\bar{x})\, \hat{\psi}^+(x') + \hat{\psi}^+(x')\, \psi(x) = \delta(x-x') \\ \hat{\psi}(x)\, \hat{\psi}(x') + \psi^*(x')\, \psi(x) = 0 \\ \psi^+(x)\, \psi^+(x') + \psi^+(x')\, \psi^+(x) = 0 \end{cases}$$

The Pauli's principle imposes then the commutation rules on the operators b_j:

$$\sum_j b_j \varphi_j(x) \sum_{j'} b_{j'}^+ \varphi_{j'}^*(x) + \sum_{j'} \hat{b}_j^+ \varphi_{j'}^*(x') \sum_j b_j \varphi_j(x) = \delta(x-x')$$

$$\Rightarrow \begin{cases} b_j b_{j'}^+ + b_{j'}^+ b_j = \delta_{jj'} \\ b_j b_{j'} + b_{j'} b_j = 0 \\ b_j^+ b_{j'}^+ + b_{j'}^+ b_j^+ = 0 \end{cases}$$

by using the orthonormality of the functions φ_j

The functions φ_j are solutions of the equation

$$H_0 \varphi_j = E_j \varphi_j$$

valid for the unperturbed atomic system.

Why we choose a different representation for Ψ? Because when we apply an $\vec{E}$-field (coherent) the atomic levels are affected and the new Hamiltonian (by property of matrices)

$$\mathcal{H}_a = \int_V \Psi^+ H_0 \Psi \, dV =$$

$$= \int \Big[\sum_j b_j^+ \varphi_j^*(\hat{x}) \, H_0 \sum_{j'} b_{j'} \varphi_{j'}(\hat{x})\Big] dV =$$

$$= \int \sum_{jj'} b_j^+ b_{j'} \, \varphi_j^*(x) \, H_0 \, \varphi_j(x) \, dV =$$

$$= \int \sum_{jj'} b_j^+ b_{j'} \, \varphi_{j'}^*(x) \, E_j \, \varphi_j(x) \, dV =$$

$$= \sum_{jj'} b_j^+ b_{j'} E_j \int \varphi_{j'}^*(x) \varphi_j(x) \, dV = \sum_{jj'} b_j^+ b_{j'} E_{j'} \delta_{jj'}$$

$$\Rightarrow \mathcal{H}_a = \sum_j E_j (b_j^+ b_j)$$

The interaction Hamiltonian is given by:

$$\mathcal{H}' = \frac{1}{2m}(\bar{p} - e\bar{A})^2 + V(r)$$

where e is the charge of the electron.

Then

$$\mathcal{H}' = \frac{1}{2m}\left(\hat{p}^2 - e\,\hat{p}\cdot\hat{A} - e\,\hat{A}\cdot\hat{p} + e^2\hat{A}^2\right) + V(r)$$

$[\hat{p}_i, \hat{A}_i]$ is not zero in principle, but applying that

$$[\hat{p}_i, \hat{F}(q_i, t)] = -i\hbar \frac{\partial F}{\partial q_i}$$

We will also neglect the term $\hat{p}^2/2m$, under the assumption that all atoms are homogeneously distributed in space, then all contributions to the field from each atom will be dephased and in average will add to zero.

Then $\mathcal{H}' = -\frac{e}{m}\vec{p}\cdot\vec{A}$

In our representation the interaction Hamiltonian will be:

$$\mathcal{H}_I = -\frac{e}{m}\int \hat{\Psi}^+(x)\,\hat{A}\,\hat{p}\,\hat{\Psi}(x)\,dV.$$

$$\bar{A}(\hat{r}) = \sum_\lambda \sqrt{\frac{\hbar}{2\varepsilon\omega_\lambda V}}\left(\hat{a}_\lambda^+ + \hat{a}_\lambda\right)A_\lambda(\hat{r}) =$$

$$= \sum_\lambda \sqrt{\frac{\hbar}{2\varepsilon\omega_\lambda V}}\left(\hat{a}_\lambda^+ e^{i\bar{k}_\lambda\cdot\bar{r}} + \hat{a}_\lambda e^{-i\bar{k}_\lambda\cdot\bar{r}}\right)$$

$$\Psi(x) = \sum_j b_j\,\varphi_j(x)$$

$$\Rightarrow \mathcal{H}_I = -\frac{e}{m}\int \sum_{j,\lambda,j'} b_j^+\,\varphi_j^*(x)\sqrt{\frac{\hbar}{2\varepsilon\omega_\lambda V}}\left(\hat{a}_\lambda^+ e^{i\bar{k}_\lambda\bar{r}} + \hat{a}_\lambda e^{-i\bar{k}_\lambda\bar{r}}\right)\hat{p}\,\times$$

$$\times\, b_{j'}^{*}\,\varphi_{j'}^{*}$$

$$\Rightarrow \mathcal{H}_I = -\frac{e}{m}\sqrt{\frac{\hbar\omega_\lambda}{2\varepsilon V}}\sum_{j\lambda j'}(b_j^+ b_{j'})\left\{\hat{a}_\lambda^+\left[\int \varphi_j^*(x)\,e^{i\bar{k}_\lambda\bar{r}}\,\hat{p}\,\varphi_{j'}(x)\right] + \right.$$

$$\left. + \hat{a}_\lambda\left[\int \varphi_j^*(x)\,e^{-i\bar{k}_\lambda\bar{r}}\,\hat{p}\,\varphi_{j'}(x)\right\}dV\right]$$

The matrix element of p ($p_{jj'}$) are:

$$p_{jj'} = m\,\dot{x}_{jj'}$$

$$= m\frac{i}{\hbar}[H, x]_{jj'} = \frac{mi}{\hbar}\left(E_j - E_{j'}\right)\hat{x}_{jj'} = i m\,\omega_{jj'}\,\hat{x}_{jj'}$$

$$\mathcal{H}_I = \frac{-e}{\cancel{m}} \sqrt{\frac{\hbar}{2\epsilon V}} \sum_{j\lambda j'} \frac{1}{\sqrt{\omega_\lambda}} \left(b_j^+ b_{j'} \right) \left(a_\lambda^+ e^{ik\bar{r}} + \hat{a}_\lambda e^{-ik\bar{r}} \right) \times$$

$$\times \int \varphi_j^*(r)\; i \cancel{m}\, \omega_{jj'}\, \hat{r}_{jj'}\, \varphi_{j'}\, dV$$

we assume $\omega_\lambda = \omega_{jj'}$

$$\mathcal{H}_I = -i \sum_{\lambda j j'} \sqrt{\frac{\hbar \omega_{jj'}}{2\epsilon V}} \left(\hat{a}_\lambda^+ e^{ik\bar{r}} + \hat{a}_\lambda e^{-ik\bar{r}} \right) \int \varphi_j^*(\hat{r})\, \underbrace{e\, \hat{r}_{jj'}}_{\text{dipole moment.}}\, \varphi_{j'}(\hat{r})\, dV$$

$$\times \left(b_j^+ b_{j'} \right)$$

The total Hamiltonian:

We are now in condition of writing the total Hamiltonian for a collection of atoms interacting with an electromagnetic field:

$$\mathcal{H} = \sum_\lambda \hbar \omega_\lambda \left(\hat{a}_\lambda^+ \hat{a}_\lambda + 1/2 \right) + \sum_j E_j \left(b_j^+ b_j \right)$$

$$- i \sum_{\lambda j j'} \sqrt{\frac{\hbar \omega_{jj'}^2}{2\epsilon V \omega_\lambda}} \cdot \langle \mu \rangle_{jj'} \left(\hat{a}_\lambda^+ \cancel{e^{ik\bar{r}}} + \hat{a}_\lambda \cancel{e^{-ik\bar{r}}} \right) \left(b_j^+ b_{j'} \right)$$

where $\langle \mu \rangle_{jj'} = \int \varphi_j^*(\hat{r})\, e\, \hat{r}\, \varphi_{j'}(\hat{r})\, dV$ are the matrix elements of the dipole moment $(e\hat{r})$.

To avoid more complex notation we did not put the sum over the atoms for the 2nd and 3rd term of the Hamiltonian.

The analysis of this multimode, multilevel and multiatom system can be considered at least "confusive". We will constraint our initial analysis to a single mode field, and a two level atom.

Attn: Discuss the problem of the factors $e^{ik\cdot\bar{r}}$ and $e^{-ik\bar{r}}$!!