Second Quantization of the Atomic Hamiltonian

We have seen that we can write the electric and magnetic field operators, and therefore the radiative parts of the Powers-Zienau-Woolley Hamiltonian, in terms of photon creation and annihilation operators. To attain some degree of symmetry, we would also like to be able to write the atomic part of this Hamiltonian in terms of raising and lowering operators, making the whole Hamiltonian simply a combination of field and atom raising and lowering operators. To begin with, let us consider the atomic Hamiltonian $\hat{H}_A$ acting on some eigenstate $|i\rangle$ with eigenvalue $\hbar\omega_i$, where $\omega_i$ has dimensions of frequency. Inserting two complete sets of these energy eigenstates around the Hamiltonian, we have

$$\hat{H}_A = \sum_i \sum_j |i\rangle \langle i| \hat{H}_A |j\rangle \langle j|.$$  

(1)

Given that the energy eigenstates are orthogonal, the expectation value of $\hat{H}_A$ becomes

$$\langle i| \hat{H}_A |j\rangle = \hbar \omega_i \delta_{ij}$$  

(2)

so that

$$\hat{H}_A = \sum_i \hbar \omega_i |i\rangle \langle i|.$$  

(3)

Note that in this case, this is simply a statement of the spectral decomposition theorem; in general, however, this process is called second quantization, where first quantization refers to the original process of finding eigenvalues and eigenvectors.

Now consider the fact that we have expressed $H_A$ in terms of projection operators. In general, one of (not necessarily diagonal) projection operators acting on another eigenstate gives

$$|i\rangle \langle j| \ell\rangle = |i\rangle \delta_{j\ell}.$$  

(4)

We can say that the projection operator has destroyed state $|\ell\rangle$ and created state $|i\rangle$ (though of course no particle has been created or destroyed here; we have merely shifted states).

Now, using this second quantization formalism, let us attack the electric dipole operator $D$. We have, inserting complete sets of energy eigenstates,

$$\hat{D} = \sum_i \sum_j |i\rangle \langle i| \hat{D} |j\rangle \langle j| \equiv \sum_i \sum_j D_{ij} |i\rangle \langle j|.$$  

(5)

As we argued before, all the diagonal matrix elements of $D$ vanish due to parity considerations. Now, using this second quantized representation of $D$, we can write the dipole Hamiltonian as

$$\hat{H}_{ED} = e \hat{D} \cdot \hat{E}_T(R)$$

$$= i e \sum_k \sum_\lambda \sum_{i,j} \left( \frac{\hbar \omega_k}{2 \epsilon_0 V} \right)^{1/2} e_{k\lambda} \cdot D_{ij} \left[ \hat{a}_{k\lambda} e^{ik \cdot R} - \hat{a}_{k\lambda}^\dagger e^{-ik \cdot R} \right] |i\rangle \langle j|.$$  

(6)

At this point, we have expressed all the parts of the atom-radiation Hamiltonian in second quantized form.

Now, let us consider a two level atom, as we have previously. We define $|1\rangle$ as the ground state, with energy $\hbar \omega_1$, and $|2\rangle$ to be the excited state, with energy $\hbar \omega_2$. We also define $\omega_0 = \omega_2 - \omega_1$. There will be two nondiagonal transition operators in system, and we define them as

$$\hat{\tau} = |1\rangle \langle 2|$$  

(7)
\[ \hat{\pi}^\dagger = |2\rangle \langle 1| . \]  

(8)

Now, setting the ground state energy to zero, the second quantized Hamiltonian is

\[ \hat{H}_A = \hbar \omega_0 |2\rangle \langle 2| = \hbar \omega_0 |1\rangle \langle 1| \langle 2| = \hbar \omega_0 \hat{\pi}^\dagger \hat{\pi} . \]  

(9)

We can also rewrite the second quantized dipole operator in terms of these transition operators:

\[ \hat{D} = D_{12}(\hat{\pi}^\dagger + \hat{\pi}) . \]  

(10)

We can now write the electric dipole Hamiltonian for this two level system as

\[ \hat{H}_{ED} = i \sum_k \sum_{\lambda} \hbar g_{k\lambda} \left[ \hat{a}_{k\lambda} e^{i k \cdot R} - \hat{a}^\dagger_{k\lambda} e^{-i k \cdot R} \right] (\hat{\pi}^\dagger + \hat{\pi}) , \]  

(11)

where

\[ g_{k\lambda} = e \left( \frac{\omega_k}{2 \epsilon_0 \hbar} \right)^{1/2} e_{k\lambda} \cdot D_{12} . \]  

(12)

If we multiply out this Hamiltonian, we get four terms; however, two of these terms do not conserve energy, so we neglect them (note that keeping these terms is necessary to explain some higher-order processes; these processes will conserve energy as a whole but not necessarily in any intermediate states). We thus rewrite the Hamiltonian as

\[ \hat{H}_{ED} = i \sum_k \sum_{\lambda} \hbar g_{k\lambda} \left[ \hat{\pi}^\dagger \hat{a}_{k\lambda} e^{i k \cdot R} - \hat{a}^\dagger_{k\lambda} \hat{\pi} e^{-i k \cdot R} \right] . \]  

(13)

If we now look at the interaction picture, where operators depend on time, we see that the neglect of the non-energy conserving terms is exactly the same rotating wave approximation we made previously, where we neglect high frequency oscillations.