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Lecture19...

Quantum Hardware – Optical Models

Class XIV

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Based on the book, Quantum Computation and Quantum Information, by M. Nielsen and I. Chuang

Optical Cavity Quantum Electrodynamics (QED) – Two-level atoms

We have discussed in previous lectures the behavior of photons and the interaction of photons together in a semiclassical non-linear medium. In this and the next lectures, we will turn our attention to atoms, their electronic structure, and their interactions with photons.

This is a very deep and well-developed field of study and we will only describe a small part of it that touches quantum computation.

- Ψ) The electronic energy eigenstates of an atom are described in box 7.6
- Ψ) In the context of quantum computation, modeling an atom as having only two states is an excellent approximation
- Ψ) This two-level atom approximation can be valid because we shall be concerned with the interaction with monochromatic light
- Ψ) In this case, the only relevant energy levels are those satisfying two conditions:
  - The energy difference between the atoms matches the energy of the incident photons (of the monochromatic field)
  - Symmetries ('selection rules') do not inhibit the transition

- Ψ) These conditions arise from basic conservation laws of energy, angular momentum, and parity
- Ψ) Since $E_n = \hbar w(n + 1/2)$, energy conservation is no more than the condition that

$$E = E_2 - E_1 = \hbar w(5/2 - 3/2) = \hbar w$$

  where E_2 and E_1 are two eigen-energies of the atom
- Ψ) Angular momentum and parity conservation requirements can be illustrated by considering the matrix element of $\hat{r}$ between two orbitals wave-functions

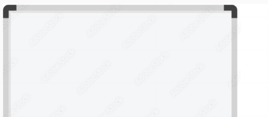
$$\langle l_1, m_1 | \hat{r} | l_2, m_2 \rangle$$

- Ψ) Without loss of generality, we can take $\hat{r}$ to be in the plane $\hat{x} - \hat{y}$, such that it can be expressed in terms of spherical harmonics (Box 7.6)

Box 7.6 Energy levels of an atom

On the whiteboard, we will study some quantum mechanical properties of atoms. Since this is a very well-studied topic, which is present in several quantum mechanical textbooks. Our intention in today's lectures is to give a basic review of this subject. For those interested, we will suggest references during the presentation where a more detailed study can be done.

WHITEBOARD



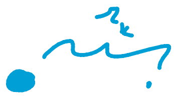
BOX 7.6 : ENERGY LEVELS OF AN ATOM

– THE ELECTRONS OF AN ATOM BEHAVE LIKE PARTICLES IN A THREE-DIMENSIONAL BOX, WITH HAMILTONIAN OF THE FORM

$$H_A = \sum \frac{|\vec{p}_k|^2}{2m} - \frac{Ze^2}{r_k} + H_{rel} + H_{ee} + H_{so} + H_{hf} \qquad (7.61)$$

- $\sum_k \frac{|p_k|^2}{2m}$ → DESCRIBES THE ELECTRONS KINETIC ENERGY
  - p_k → MOMENTUM OF ELECTRON k
  - m → ELECTRON MASS

- $-\frac{Ze^2}{r_k}$ → COULOMBIAN ATTRACTION BETWEEN THE ELECTRON $(-e)$ AND THE NUCLEUS
  - r_k → POSITION OF ELECTRON k



  - Z → ATOMIC NUMBER

- H_{rel} → RELATIVISTIC CORRECTION TERM

$$E^2 = (pc)^2 + m^2c^4 \Rightarrow E = \sqrt{p^2c^2 + m^2c^4} = c\sqrt{p^2 + m^2c^2}$$

$$E = mc^2\sqrt{\frac{p^2}{m^2c^2} + 1} \simeq mc^2\left(1 + \frac{1}{2}\frac{p^2}{m^2c^2} - \frac{p^4}{8m^4c^4} + \cdots\right) \qquad p = mv, \quad v \ll c$$

$$E \simeq mc^2 + \frac{p^2}{\ldots} - p^4 \ldots$$

. . . / $v \ll c$

$$E \simeq \underbrace{mc^2}_{\text{"REST MASS"}} + \underbrace{\frac{p^2}{2m}}_{\text{KINETIC ENERGY}} - \underbrace{\frac{p^4}{8m^3c^2}}_{\text{RELATIVISTIC CORRECTION}} + \cdots$$

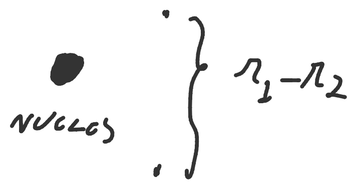
$$H_{rel} \simeq -\frac{p^4}{8m^3c^2}$$

$$\rightarrow \frac{H_{rel}}{H_K} = \frac{p^4/8m^3c^2}{p^2/2m} = \frac{1}{4}\left(\frac{v^2}{c^2}\right) \simeq \left(\frac{1}{137}\right)^2 \simeq \alpha^2$$ (HYDROGEN ATOM)

- $H_{ee} \rightarrow$ DESCRIBES ELECTRON-ELECTRON COUPLINGS

EXAMPLE: HELIUM ATOMS

$$H_{ee} \simeq \frac{e^2}{|r_1 - r_2|}$$



- $H_{SO} \rightarrow$ SPIN-ORBIT INTERACTION, WHICH CAN BE INTERPRETED AS THE SPIN OF THE ELECTRON INTERACTING WITH A MAGNETIC FIELD GENERATED BY ITS ORBIT AROUND THE ATOM

$$H_{SO} \simeq \frac{e^2}{m^2c^2}\frac{1}{r^3}\vec{L}\cdot\vec{S}$$

→ PHYSICAL ORIGIN OF H_{SO}

$v = \frac{p}{m}$, VELOCITY OF THE ELECTRON IN THE ELECTROSTATIC FIELD E CREATED BY THE

PROTON

— IT SHOULD APPEARS IN THE ELECTRON REFERENCE FRAME A MAGNETIC FIELD

$$\vec{B} = -\frac{1}{c^2}\vec{v} \times \vec{E}$$

— SINCE THE ELECTRON POSSESSES AN INTRINSIC MAGNETIC MOMENT

$$\vec{\mu}_s = \frac{q\vec{S}}{m}$$

IT INTERACTS WITH $\vec{B}$, GIVEN THE CORRESPONDING INTERACTION ENERGY

$$E_{SO} = H_{SO} = -\vec{\mu}_s \cdot \vec{B}$$

$$H_{SO} = -\frac{q\vec{S}}{m} \cdot \left(-\frac{1}{c^2}\vec{v} \times \vec{E}\right)$$

BUT $\vec{E} = -\frac{1}{q}\frac{dV_e(\vec{r})}{dr}\frac{\vec{r}}{r}$, $V_e = -\frac{e^2}{r}$

$$H_{SO} = -\frac{q\vec{S}}{m} \cdot \left[-\frac{1}{c^2}\vec{v} \times \left(-\frac{1}{q}\frac{dV}{dr}\frac{\vec{r}}{r}\right)\right] = \frac{\cancel{q}\vec{S}}{m} \cdot \left[\frac{1}{\cancel{q}c^2}\frac{dV}{dr}\vec{v} \times \frac{\vec{r}}{r}\right]$$

$\vec{v} = \frac{\vec{p}}{m}$

$$H_{SO} = \frac{1}{mrc^2}\frac{dV}{dr}\vec{S} \cdot \left(\frac{\vec{p}}{m} \times \vec{r}\right) = \frac{1}{m^2c^2r}\frac{dV}{dr}\vec{S} \cdot \vec{L}$$

AND $V = -\frac{e^2}{r} \Rightarrow \frac{dV}{dr} = \frac{e^2}{r^2}$

$$H_{SO} = \frac{e^2}{m^2c^2r^3}\vec{L} \cdot \vec{S}$$

MAGNITUDE: $\dfrac{H_{SO}}{H_e} \simeq \dfrac{e^2\, \vec{L}\cdot\vec{S}/m^2c^2r^3}{e^2/r}$, $\vec{L}\cdot\vec{S} \simeq \hbar^2$

$$\frac{H_{SO}}{H_e} \simeq \frac{e^2\hbar^2/m^2c^2r^3}{e^2/r} = \frac{\hbar^2}{m^2c^2r^2} \quad , \quad r \simeq \frac{\hbar^2}{me^2} \rightarrow \text{BOHR RADIUS}$$

$$\frac{H_{SO}}{H_e} \simeq \frac{e^4}{\hbar^2c^2} = \alpha^2 = \left(\frac{1}{137}\right)^2$$

- H_{hf} → IS THE HYPERFINE INTERACTION, WHICH CAN BE INTERPRETED AS THE SPIN OF THE ELECTRON INTERACTING WITH THE MAGNETIC FIELD GENERATED BY NUCLEUS

$$\frac{H_{hf}}{H_K} \sim \alpha^2 = \left(\frac{1}{137}\right)^2$$

<u>ANOTHER TYPE OF CORRECTIONS</u>

- H_{SS} → $H_S = \dfrac{\vec{\mu}_e\cdot\vec{\mu}_p - 3(\vec{\mu}_e\cdot\hat{r})(\vec{\mu}_p\cdot\hat{r})}{r^3}$, $\hat{r} = \dfrac{\vec{r}}{r}$

- LAMB-SHIFT: THE CORRECTION THAT COMES FROM VACUUM FLUCTUATIONS FROM AN QUANTIZED EM FIELD

$$H_{LAMB} \simeq \frac{mc^2 Z^4 \alpha^5}{n^3} \ll H_K$$

REFERENCES: COHEN

GASIOROWICZ (QUANTUM PHYSICS)

→ LET'S DISCUSS THE MAIN STEPS FROM THE SOLUTION OF THE SCHRODINGER EQUATION FOR HYDROGEN TYPE ATOMS

1. $H_A \Psi(r,\theta,\varphi) = -\beta \nabla^2_{r,\theta,\varphi} \Psi(r,\theta,\varphi) + V(r)\Psi(r,\theta,\varphi) = E\Psi(r,\theta,\varphi)$

$\beta = \dfrac{\hbar^2}{2\mu}$ / $\mu = \dfrac{m_p + m_e}{m_p m_e}$ → REDUCED MASS

2. $\nabla^2_{r,\theta,\varphi} = \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2\dfrac{\partial}{\partial r}\right) + \dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right) + \dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\varphi^2}$

3. $\Psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$

4. USE (3) AND (2) IN (1) TO OBTAIN ONE RADIAL AND ONE ANGULAR EQUATION

a) $\dfrac{1}{\beta R}\dfrac{d}{dr}\left[r^2\dfrac{dR(r)}{dr}\right] + \dfrac{1}{\alpha}\left(E - V(r)\right) = \lambda$ (COHEN 790)

b) $\dfrac{1}{Y\sin\theta}\dfrac{\partial}{\partial\theta}\left[\sin\theta\dfrac{\partial Y(\theta,\varphi)}{\partial\theta}\right] + \dfrac{1}{Y}\dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\varphi^2}Y(\theta,\varphi) = \lambda = \ell(\ell+1)$

(COHEN 662)

THE SOLUTION FROM THE RADIAL EQUATION

$$R_{nl}(r) = e^{-r/n\beta}\left(\frac{r}{\beta}\right)^{l} G_{nl}\left(\frac{r}{\beta}\right)$$

$G_{nl} \rightarrow$ ARE POLYNOMIALS FROM $\frac{r}{\beta}$

$$n = l+1,\ l+2,\ l+3,\ \ldots$$

5. $Y(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$, using in (46)

a) $$\frac{1}{\Phi}\frac{d^2\Phi(\varphi)}{d\varphi^2} = -m^2 \Rightarrow \Phi_m(\varphi) = A\,e^{im\varphi}$$

b) $$-\frac{1}{\Theta}\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \lambda\sin^2\theta = -m^2$$

$\lambda \rightarrow l(l+1)$

$$\Theta_{lm}(\theta) = \sin^{|m|}\theta\; P_{l|m|}(\cos\theta)$$

$$m = 0, 1, 2, 3, \ldots$$

$$l = |m|,\ |m|+1,\ |m|+2,\ \ldots$$

$$\rightarrow Y_{lm}(\theta,\varphi) = \Theta_{lm}\,\Phi_m = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\,P_{lm}(\cos\theta)\,e^{im\varphi} \quad (7.63)$$

$$\rightarrow P_{lm}(x) = \frac{(1-x^2)^{m/2}}{2^l\,l!}\frac{d^{m+l}}{dx^{m+l}}(x^2-1)^l \quad (7.64)$$

$P_{\ell m} \to$ LEGENDRE FUNCTIONS

$Y_{\ell m} \to$ SPHERICAL HARMONICS

PROPERTIES : COHEN PAGS 664-665 AND PAGS 678-689

- PARITY AND ROTATIONS

$$r \to r \,, \quad \theta \to \pi - \theta \,, \quad \varphi = \pi + \varphi$$

- ORTHONORMALIZATION AND CLOSURE RELATIONS

$$\int_0^{2\pi} d\varphi \int_0^{\pi} \operatorname{sen}\theta \; Y^*_{\ell' m'}(\theta,\varphi) \, Y_{\ell m}(\theta,\varphi) = \delta_{\ell'\ell}\,\delta_{m'm}$$

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta,\varphi)\, Y^*_{\ell m}(\theta',\varphi') = \frac{1}{\operatorname{sen}\theta}\,\delta(\theta-\theta')\,\delta(\varphi-\varphi')$$