Equation Format

Reference:C:\Users\Franc\new folder\Physical Constants.xmcd

Reference:C:\Users\Franc\new folder\unit vectors.xmcd

1
INTERACTION EM FIELD-CRYSTAL

A crystal is a well ordered system composed by the same atoms or molecules, they are spatially arranged so as to form a regular lattice and where it is possible to identify an elementary cell. Crystals can be: good conductors, semiconductors and isolators as th quartz crystal. (Using an energy-band model of the crystal, there prevail the valence energy band and the conduction energy band) One verify that in a good conductor the two bands overlap and the electromagnetic field is reflected on its surface.
If the electromagnetic field is polarized, the electric field vector undergoes a reflection of 180° so that, on the metallic surface the electric field vector is null. In the same point, instead, the magnetic component of the field doubles. Indeed there is no electromagnetic propagation in metals. In a semiconductor, however, there is a limited gap between the two bands, while in an insulator the energy gap is much greater than that of a semiconductor). A dielectric, instead, is an isolator, it can be a non conducting crystal but also a disordered system of atoms or molecules (no lattice) for example an amorphous substance (formed by some organic molecules carbon compounds, or polymers) or glass formed, for example, by non crystallized silicon dioxide. Th electromagnetic field propagates through semiconductors and dielectrics. In the following pages, it will be analyzed the interactio between a polarized electromagnetic field propagating through the crystal. As will be seen, the propagation occur only within a certain frequency band of the EM field, this band depends on the medium in which the EM wave propagates. (In other words there are crystals transparent to the visible light, other are opaque to the visible light but transparent at infrared frequency (Ge, Si and so on).

(Vectors depending from time and position, are written in ***bold blue*** *fonts, while vectors depending only from the position* ***r*** *are written in* ***bold light blue*** *fonts).*

Unit of measure

EM Field vectors' units of measure

Magnetic induction **B** unit measure is: $T = \frac{Wb}{m^2} = \frac{H}{m} \cdot \frac{A}{m}$ $\quad 1 \cdot \frac{Wb}{m^2} = 1\,T$ $\quad 1 \cdot T = 1 \cdot \frac{H}{m^2} \cdot A$

Magnetic field intensity **H**: $\frac{A}{m} = 1 \cdot \frac{Wb}{m \cdot H}$ $\quad Oe = 79.577\,\frac{A}{m}$ $\quad 1 \cdot \frac{A}{cm} = 1.26 \cdot Oe$

Electric field intensity **E**: $\frac{volt}{m} = 1 \cdot \frac{Wb}{m \cdot s}$ $\quad \frac{volt}{m} = 1 \cdot \frac{T \cdot m}{s}$ $\quad \frac{volt}{m} = 12.566 \cdot \frac{Oe \cdot mH}{s}$

Dielectric constant of the vacuum: $\varepsilon_0 = 8.854 \cdot \frac{pF}{m}$

Magnetic permeability of the vacuum $\mu_0 = 1.257 \cdot \frac{\mu H}{m}$ $\quad \frac{\mu H}{m} = 79.577 \cdot \frac{\mu T}{Oe}$ $\quad \mu_0 = 100 \cdot \frac{\mu T}{Oe}$

Electron charge: $q_e = 1.602 \times 10^{-19}\,C$

Electric displacement **D**: $\frac{F}{m} \cdot \frac{volt}{m} = 1\,\frac{A \cdot s}{m^2}$

Electric current density $\mathbf{J}_\sigma$: $\frac{A}{m^2}$

Magnetic current density $\mathbf{J}_\mathbf{m}$: $\frac{V}{m^2} = \frac{Wb}{m^2 \cdot s} = \frac{T}{s}$ $\quad 1 \cdot \frac{V}{m^2} = 1 \cdot \frac{T}{s}$ $\quad 1 \cdot \frac{V}{m^2} = 1 \cdot \frac{Wb}{m^2 \cdot s}$

Unit of measure of the Magnetic vector potential **A**

. If you choose (Electromagnetics, **Option 1)**) $\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$, unit of measure: $[\ \mathbf{A}\ ] = \frac{Wb}{m}$.

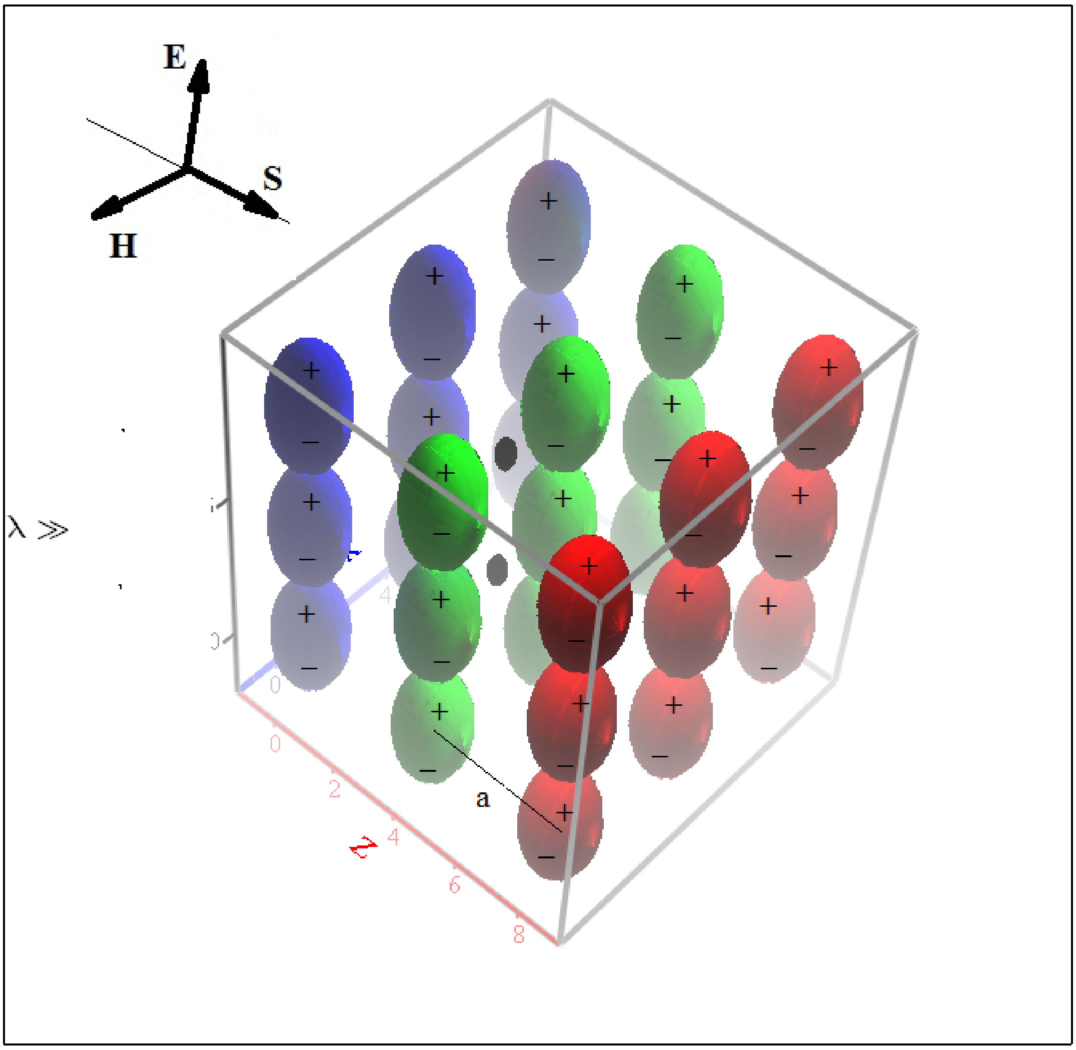
If you choose (Electromagnetics, **Option 2)**) $\mathbf{H}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$, then the unit of measure is $[\ \mathbf{A}\ ] =$ Ampère.

Unit of measure

Electric field

Dipole approximation

Spheres



Dipoles in a crystal lattice $\lambda \gg a$

The electric field is linked to the vector potential by the relation a6):

$$\frac{\text{volt}}{\text{m}} \quad \boxed{\mathbf{E}(\mathbf{r},t) = -\nabla\,\varphi(\mathbf{r},t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t)} \quad \frac{\text{Wb}}{\text{m}\cdot\text{s}} = 1\cdot\frac{\text{volt}}{\text{m}} \qquad 3)$$

$$\text{if } \varphi(\mathbf{r},t) = \text{constant}, \boxed{\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t)}$$

furthermore the time derivative of the vector potential can be rewritten as the following scalar product:

$$\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t) = \frac{\partial}{\partial \mathbf{r}}\mathbf{A}(\mathbf{r},t)\cdot\frac{\partial}{\partial t}\mathbf{r} = \mathbf{v}\cdot\nabla\,\mathbf{A}(\mathbf{r},t) \qquad 4)$$

A(r,t) time derivative

where $\mathbf{r}$ is the position, at time t, of the vector potential.

$$\text{if } \varphi(\mathbf{r},t) = \text{constant}, \boxed{\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t) = -\mathbf{v}\cdot\nabla\,\mathbf{A}(\mathbf{r},t)} \qquad 5)$$

unites of measure

Considering the propagation of time harmonic fields, the vector $\mathbf{v}$ is the speed of the EM field through the lattice, namely slightly less than the light speed c, that is $|\mathbf{v}| = \frac{c}{\eta}$, where η is the refraction index of the crystal. The propagation direction, for time harmonic field, is that of the wave vector $\mathbf{k}$ with unit vector $\frac{\mathbf{k}}{|\mathbf{k}|}$ orthogonal to $\mathbf{A}(\mathbf{r},$

Namely $\mathbf{v} = \frac{c}{\eta} \cdot \frac{\mathbf{k}}{|\mathbf{k}|}$. 6)

A, E, H

Substituting 4) in 3) I get: $\mathbf{E}(\mathbf{r},t) = -\nabla\,\varphi(\mathbf{r},t) - \mathbf{v}\cdot\nabla\,\mathbf{A}(\mathbf{r},t)$ 7)

unites of measure

furthermore, collecting the gradient operators, considering $\mathbf{v}$ constant, I can write:

$$\mathbf{E}(\mathbf{r},t) = -\nabla\left(\varphi(\mathbf{r},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{r},t)\right) = -\nabla\,(\Phi) \qquad 8)$$

so that I can define the scalar potential: $\boxed{\Phi(\mathbf{r},t) = \varphi(\mathbf{r},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{r},t)}$ $\mathbf{v}$ constant 9)

while the potential energy is $U(\mathbf{r},t) = -q_e\cdot\left(\varphi(\mathbf{r},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{r},t)\right)$ $q_e = 1.602\times10^{-19}\,C$ 10)

which is useful to define the Lagrangian (see below).

$$\text{if } \varphi(\mathbf{r},t) = \text{constant},\ \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t) = -\mathbf{v}\cdot\nabla\,\mathbf{A}(\mathbf{r},t)$$

$$\Phi(\mathbf{r},t) = \mathbf{v}\cdot\mathbf{A}(\mathbf{r},t)$$

$$U(\mathbf{r},t) = -q_e\cdot\mathbf{v}\cdot\mathbf{A}(\mathbf{r},t) \qquad \mathbf{v}\ \text{constant}$$

All that I've sad till now is related to the electromagnetic field. But, to study the interactions wave-materials, I have know the dynamics of one atom of the crystal lattice that, subjected to a em field whose wavelength λ is much greate than the reticular constant, here indicated with letter a, causes the single atom to behave like a dipole.

Taylor series of the EM vector potential A (moving at light speed)

Lagrange equations system

Approximations for small movements

Example: System with two degree of freedom

The Lagrangian within the Gauss System

Consider as Lagrangian coordinates, the position q, and the momentum $p = m\cdot q'$, $q' = v$.

Electric potential at q: $\varphi(q,t)$, while the potential energy is $U(q,t) = -q_e\cdot\left(\varphi(q,t) + \mathbf{q'}\cdot\mathbf{A}(\mathbf{r},t)\right)$

The Lagrangian of the system I deal with is:

$q_e = 1.602\times10^{-19}\,C$ $\mathscr{L}(q,q',t) = \frac{1}{2}\cdot p\cdot q' + q_e\cdot\varphi(q) + q_e\cdot\mathbf{q'}\cdot\mathbf{A}(\mathbf{r},t)$ 11)

For one dipole's electron, the Lagrange equation is: $\frac{d}{dt}\frac{\partial}{\partial\mathbf{q'}}\mathscr{L}(\mathbf{q},\mathbf{q'},t) - \frac{\partial}{\partial\mathbf{q}}\mathscr{L}(\mathbf{q},\mathbf{q'},t) = 0$ 12)

Remark:

If I define the new Lagrangian $\mathscr{L}_1(\mathbf{q},\mathbf{q'},t) = \mathscr{L}(\mathbf{q},\mathbf{q'},t) + f(t)$, the differential equation doesn't varies, indeed:

$$\frac{d}{dt}\frac{\partial}{\partial\mathbf{q'}}\left(\mathscr{L}(\mathbf{q},\mathbf{q'},t) + f(t)\right) - \frac{\partial}{\partial\mathbf{q}}\left(\mathscr{L}(\mathbf{q},\mathbf{q'},t) + f(t)\right) = \frac{d}{dt}\frac{\partial}{\partial\mathbf{q'}}\mathscr{L}(\mathbf{q},\mathbf{q'},t) - \frac{\partial}{\partial\mathbf{q}}\mathscr{L}(\mathbf{q},\mathbf{q'},t) \qquad 13)$$

since f(t) isn't a function of $\mathbf{q}$ and $\mathbf{q'}$ $\frac{\partial}{\partial\mathbf{q'}}f(t) = 0$ and $\frac{\partial}{\partial\mathbf{q}}f(t) = 0$

Accordingly I can add, to the Lagrangian $\mathscr{L}$, the arbitrary, but useful term $-q_e\cdot\frac{\partial}{\partial t}\left(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)\right)$ without affecting the analysis of the dynamic behavior of the system (because q is almost constant and A vary very slowly in space, it follows that the result is a function of the time only so that $\frac{\partial}{\partial q'}\frac{\partial}{\partial t}\left(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)\right) = 0$ and $\frac{\partial}{\partial q}\frac{\partial}{\partial t}\left(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)\right) = 0$.

I can write: $$\mathscr{L}_{1}(\mathbf{q},\mathbf{q'},t) = \mathscr{L}(\mathbf{q},\mathbf{q'},t) - q_e\cdot\frac{\partial}{\partial t}\left(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)\right) \tag{14}$$

after a substitution of 11) $$\mathscr{L}_{1}(\mathbf{q},\mathbf{q'},t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} + q_e\cdot V(\mathbf{q}) + q_e\cdot\mathbf{q'}\cdot\mathbf{A}(\mathbf{q},t) - q_e\cdot\frac{\partial}{\partial t}\left(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)\right) \tag{15}$$

the partial derivatives is $$\frac{\partial}{\partial t}\left(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)\right) = \mathbf{A}(\mathbf{q},t)\cdot\mathbf{q'} + \mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t) \tag{16}$$

which substituted in 15) gives:

$$\mathscr{L}_{1}(\mathbf{q},\mathbf{q'},t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} + q_e\cdot V(\mathbf{q}) + q_e\cdot\mathbf{q'}\cdot\mathbf{A}(\mathbf{q},t) - q_e\cdot\left(\mathbf{A}(\mathbf{q},t)\cdot\mathbf{q'} + \mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)\right) \tag{17}$$

or $$\mathscr{L}_{1}(\mathbf{q},\mathbf{q'},t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} + q_e\cdot V(\mathbf{q}) + q_e\cdot\mathbf{q'}\cdot\mathbf{A}(\mathbf{q},t) - q_e\cdot\mathbf{A}(\mathbf{q},t)\cdot\mathbf{q'} - q_e\cdot\mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t) \tag{18}$$

simplifying, I get: $$\mathscr{L}_{1}(\mathbf{q},\mathbf{q'},t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} + q_e\cdot V(\mathbf{q}) - q_e\cdot\mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t) \tag{19}$$

Consider an EM ***plane wave*** propagating through the crystal along a path aligned with the optical axis z. This implie that the electromagnetic field is orthogonal to the z propagation direction. As a result I indicate the electric field as transversal:

$$\boxed{\mathbf{E_T}(\mathbf{q},t) = -\nabla\varphi(\mathbf{q},t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)}$$

which, for a space constant potential φ, simplify to:

$$\boxed{\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t) = -\mathbf{E_T}(\mathbf{q},t)} \text{ transversal electric field intensity} \tag{20}$$

$$\mathbf{E_T}(\mathbf{q},t) = E_x(x,y,z,t)\cdot\mathbf{i_x} + E_y(x,y,z,t)\cdot\mathbf{i_y} + 0\cdot\mathbf{i_z}$$

the Lagrangian 19), finally, is: $$\boxed{\mathscr{L}_{1}(\mathbf{q},\mathbf{q'},t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} + q_e\cdot V(\mathbf{q}) + q_e\cdot\mathbf{q}\cdot\mathbf{E_T}(\mathbf{q},t)} \tag{21}$$

Time harmonic Field decomposition

for n electrons I get: $$\mathscr{L}_{1} = \frac{1}{2}\cdot\sum_{i=1}^{n}\left(\mathbf{p_i}\cdot\mathbf{q'_i}\right) + q_e\cdot\sum_{i=1}^{n}V(\mathbf{q_i}) + q_e\cdot\sum_{i=1}^{n}\left(\mathbf{q_i}\cdot\mathbf{E_T}(\mathbf{q},t)\right) \tag{22}$$

The modified Lagrangian correspondingly is:

$$\boxed{\mathscr{L}_{1} = \sum_{i=1}^{n}\left[\frac{1}{2}\cdot\left(\mathbf{p_i}\cdot\mathbf{q'_i}\right) + q_e\cdot V(\mathbf{q_i}) + q_e\cdot\mathbf{q_i}\cdot\mathbf{E_T}(\mathbf{q},t)\right]} \tag{23}$$

For one particle with electric charge Q, I get:

$$U(\mathbf{q},t) = Q\cdot\left(\varphi(\mathbf{q},t) + \mathbf{q'}\cdot\mathbf{A}(\mathbf{q},t)\right)$$

$$\mathscr{L}(\mathbf{q},\mathbf{q'},t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - Q\cdot V(\mathbf{q}) - Q\cdot\mathbf{q'}\cdot\mathbf{A}(\mathbf{q},t)$$

$$\mathscr{L}_1(\mathbf{q},\mathbf{q}',t) = \mathscr{L}(\mathbf{q},\mathbf{q}',t) + Q\cdot\frac{\partial}{\partial t}(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t))$$

$$\mathscr{L}_1(\mathbf{q},\mathbf{q}',t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q}' - Q\cdot V(\mathbf{q}) - Q\cdot\mathbf{q}'\cdot\mathbf{A}(\mathbf{q},t) + Q\cdot\frac{\partial}{\partial t}(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t))$$

$$\frac{\partial}{\partial t}(\mathbf{q}\cdot\mathbf{A}(\mathbf{q},t)) = \mathbf{A}(\mathbf{q},t)\cdot\mathbf{q}' + \mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)$$

$$\mathscr{L}_1(\mathbf{q},\mathbf{q}',t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q}' - Q\cdot V(\mathbf{q}) - Q\cdot\mathbf{q}'\cdot\mathbf{A}(\mathbf{q},t) + Q\cdot\left(\mathbf{A}(\mathbf{q},t)\cdot\mathbf{q}' + \mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)\right)$$

$$\mathscr{L}_1(\mathbf{q},\mathbf{q}',t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q}' - Q\cdot V(\mathbf{q}) - Q\cdot\mathbf{q}'\cdot\mathbf{A}(\mathbf{q},t) + Q\cdot\mathbf{A}(\mathbf{q},t)\cdot\mathbf{q}' + Q\cdot\mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)$$

$$\mathscr{L}_1(\mathbf{q},\mathbf{q}',t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q}' - Q\cdot V(\mathbf{q}) + Q\cdot\mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)$$

$$\boxed{\mathbf{E_T}(\mathbf{q},t) = -\nabla V(\mathbf{q},t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t)}$$

which, for a constant potential V, simplify to:

$$\frac{\partial}{\partial t}\mathbf{A}(\mathbf{q},t) = -\mathbf{E_T}(\mathbf{q},t)$$

$$\mathbf{E_T}(\mathbf{q},t) = E_x(x,y,z,t)\cdot\mathbf{i_x} + E_y(x,y,z,t)\cdot\mathbf{i_y} \qquad E_z(x,y,z,t) = 0$$

$$\boxed{\mathscr{L}_1(\mathbf{q},\mathbf{q}',t) = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q}' - Q\cdot V(\mathbf{q}) - Q\cdot\mathbf{q}\cdot\mathbf{E_T}(\mathbf{q},t)}$$

for n particles with electric charge Q, I get:

$$\boxed{\mathscr{L}_1 = \sum_{i=1}^{n}\left[\frac{1}{2}\cdot(p_i\cdot q'_i) - Q\cdot V(\mathbf{q_i}) - Q\cdot\mathbf{q_i}\cdot\mathbf{E_T}(\mathbf{q},t)\right]}$$

Hamiltonian's calculation

Hamilton equations

Classical Hamilton equations

Kinetic energy : T
Potential energy : U

Hamiltonian : $\mathscr{H}\left(q_1, q_2, ...q_n, p_1, p_2, ...p_n, t\right) = T + U = 2\cdot T - \mathscr{L}\left(q_1, q_2, ...q_n, q'_1, q'_{2.n}, ...q', t\right)$

$$\mathscr{H} = \frac{1}{2}\cdot\sum_{i=1}^{n}\left(p_i\cdot q'_i\right) + U$$

$$\mathscr{L} = \frac{1}{2}\cdot\sum_{i=1}^{n}\left(p_i\cdot q'_i\right) - U$$

$$\mathscr{H} = 2\cdot T - \mathscr{L} = 2\cdot\frac{1}{2}\cdot\sum_{i=1}^{n}\left(p_i\cdot q'_i\right) - \mathscr{L} = \sum_{i=1}^{n}\left(p_i\cdot q'_i\right) - \mathscr{L} = \sum_{i=1}^{n}\left(q'_i\cdot\frac{\partial}{\partial q'_i}\mathscr{L}\right) - \mathscr{L}$$

The conjugated momenta can be written as functions of the Lagrangian $p_i = \frac{\partial}{\partial q'_i}\mathscr{L}$, $i = 1, 2, 3 .. n$

$$\mathscr{H} = \sum_{i=1}^{n}\left(p_i\cdot q'_i\right) - \mathscr{L} = \sum_{i=1}^{n}\left(q'_i\cdot\frac{\partial}{\partial q'_i}\mathscr{L}\right) - \mathscr{L}$$

$$\mathscr{H} = \sum_{i=1}^{n}\left(q'_i\cdot\frac{\partial}{\partial q'_i}\mathscr{L}\right) - \mathscr{L}$$

Hamilton equations: $\boxed{q'_i = \frac{\partial}{\partial p_i}\mathscr{H}}$ $i = 1, 2, 3 .. n$

$$\boxed{p'_i = -\frac{\partial}{\partial q_i}\mathscr{H}}$$

Hamilton equations

For one electron, the Hamiltonian is: $\mathscr{H} = \mathbf{p}\cdot\mathbf{q'} - \mathscr{L}_1 = \mathbf{p}\cdot\mathbf{q'} - \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - q_e\cdot V(\mathbf{q}) - q_e\cdot\mathbf{q}\cdot\mathbf{E_T}(\mathbf{q}, t)$ 24)

namely: $\mathscr{H} = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - q_e\cdot V(\mathbf{q}) - q_e\cdot\mathbf{q}\cdot\mathbf{E_T}(\mathbf{q}, t)$ 25)

The effect of the electromagnetic field acting on the crystal, is the polarization of each atom or molecule part of it.

The electric dipole

Define the *dipole moment* as: $\boxed{\boldsymbol{\mu} = -q_e\cdot\mathbf{d}}$, which, substituted in the previous equation 25), yields:

$$\boxed{\mathscr{H} = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - q_e\cdot V(\mathbf{q}) + \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q}, t)} \quad 27)$$

(μ and $\mathbf{E_T}$ are aligned only for isotropic materials) In this relation (27)) I distinguish three Hamiltonians:

Unperturbed Hamiltonian: $\mathscr{H}_0 = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q}'$ 28)

Relaxation Hamiltonian: $\mathscr{H}_r = -q_e\cdot V(\mathbf{q})$ 29)

Interaction Hamiltonian: $\mathscr{H}_1 = \mu\cdot\mathbf{E_T}(\mathbf{q},t)$ 30)

that is: $\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_1 + \mathscr{H}_r$ 31)

Define the dipole moment ***for n atoms or molecules*** as: $\boxed{\mu_1 = -\sum_{i=1}^{n}\left(q_{e_i}\cdot\mathbf{d}_i\right)}$ $(C\cdot m)$ 32)

So that the Hamiltonian is:

$$\mathscr{H} = \sum_{i=1}^{n}\left[\frac{1}{2}\cdot(p_i\cdot q'_i)\right] - \sum_{i=1}^{n}\left(q_e\cdot V(q_i)\right) + \mu_1\cdot\mathbf{E_T}(q,t) \quad 33)$$

the resulting electric potential energy is $q_e\cdot V(q_1,q_2,..,q_n) = \sum_{i=1}^{n}\left(q_e\cdot V(q_i)\right)$

that is: $$\boxed{\mathscr{H} = \frac{1}{2}\cdot\sum_{i=1}^{n}(p_i\cdot q'_i) - q_e\cdot V(q_1,q_2,..,q_n) + \mu_1\cdot\mathbf{E_T}(q,t)} \quad 34)$$

Quadrupole approximation of the vector potential

Quadrupole approximation of the vector potential

I Rewrite the Taylor series of the vector potential but now I trunk the series to the first order term:

$$\mathbf{A}(\mathbf{q},t) = \mathbf{A}(\mathbf{r}+\mathbf{R},t) = \left[\mathbf{A}(\mathbf{R},t) + \sum_{k=1}^{\infty}\left[\frac{1}{k!}\cdot(\mathbf{r}\cdot\nabla)\cdot\mathbf{A}\right]^k\right] \approx \left[\mathbf{A}(\mathbf{R},t) + (\mathbf{r}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right] \quad 35)$$

$$[\ \mathbf{A}\ ] = \frac{Wb}{m}$$

namely: $$\mathbf{A}(\mathbf{q},t) = \mathbf{A}(\mathbf{r}+\mathbf{R},t) \approx \left[\mathbf{A}(\mathbf{r},t) + (\mathbf{r}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right] \quad 36)$$

then I substitute it in the equation of the electric field 3) namely:

$$\boxed{\mathbf{E}(\mathbf{r},t) = -\nabla\,\varphi(\mathbf{r},t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t)}$$

$$\mathbf{E}(\mathbf{r},t) = -\nabla\left[\varphi(\mathbf{r},t) + \mathbf{v}\cdot\left[\mathbf{A}(\mathbf{r},t) + (\mathbf{r}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right]\right] = -\nabla\,(U) \quad 37)$$

$$\boxed{\Phi_1(\mathbf{r},t) = \varphi(\mathbf{r},t) + \mathbf{v}\cdot\left[\mathbf{A}(\mathbf{r},t) + (\mathbf{r}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right]} \quad 38)$$

Scalar potential $\varphi(\mathbf{r},t) + \mathbf{v}\cdot\left[\mathbf{A}(\mathbf{r},t) + (\mathbf{r}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right]$ 39) potential energy $\quad U(\mathbf{r},t) = -q_e\cdot\Phi_1 = -q_e\cdot\varphi(\mathbf{r},t) + \mathbf{v}\cdot\left[\mathbf{A}(\mathbf{r},t) + (\mathbf{r}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right]$ 40)

The Lagrangian of n particles is:

$$\boxed{\mathscr{L} = \frac{1}{2}\cdot\sum_{i=1}^{n}\left(p_i\cdot q'_i\right) - U} \qquad 41)$$

(q_i is the ith position and q_e the electron charge)

The Lagrangian of the system I deal with is:

$$V(q) = \Phi(x,y,z,t) \quad \mathscr{L}(q,q',t) = \frac{1}{2}\cdot p\cdot q' + q_e\cdot V(q) - q_e\cdot q'\cdot\left[\mathbf{A}(\mathbf{r},t) + (\mathbf{q}\cdot\nabla)\cdot\mathbf{A}(\mathbf{r},t)\right] \qquad \mathbf{q} = \mathbf{r} \qquad 42)$$

$$\mathbf{q}\cdot\nabla = \left(x\cdot\mathbf{i_x} + y\cdot\mathbf{i_y} + z\cdot\mathbf{i_z}\right)\cdot\left(\mathbf{i_x}\cdot\frac{\partial}{\partial x} + \mathbf{i_y}\cdot\frac{\partial}{\partial y} + \mathbf{i_z}\cdot\frac{\partial}{\partial z}\right) = x\cdot\frac{\partial}{\partial x} + y\cdot\frac{\partial}{\partial y} + z\cdot\frac{\partial}{\partial z} \qquad 43)$$

$$(\mathbf{q}\cdot\nabla)\cdot\mathbf{A} = \left(x\cdot\frac{\partial}{\partial x} + y\cdot\frac{\partial}{\partial y} + z\cdot\frac{\partial}{\partial z}\right)\cdot\mathbf{A} \qquad 44)$$

$$\left(x\cdot\frac{\partial}{\partial x} + y\cdot\frac{\partial}{\partial y} + z\cdot\frac{\partial}{\partial z}\right)\cdot\mathbf{A} = \left(x\cdot\frac{\partial}{\partial x}A_x + y\cdot\frac{\partial}{\partial y}A_x + z\cdot\frac{\partial}{\partial z}A_x\right)\cdot\mathbf{i_x} \ldots$$
$$+\left(x\cdot\frac{\partial}{\partial x}A_y + y\cdot\frac{\partial}{\partial y}A_y + z\cdot\frac{\partial}{\partial z}A_y\right)\cdot\mathbf{i_y} \ldots$$
$$+\left(x\cdot\frac{\partial}{\partial x}A_z + y\cdot\frac{\partial}{\partial y}A_z + z\cdot\frac{\partial}{\partial z}A_z\right)\cdot\mathbf{i_z}$$

Quadrupole approximation of the vector potential

Quadrupole Hamiltonian

$$\boxed{\mathscr{H} = \frac{1}{2}\cdot p\cdot q' - q_e\cdot V(q) - \mu\cdot\mathbf{E_T}(\mathbf{r},t) - \mathbf{M}\cdot\mathbf{B} + \frac{1}{2}\cdot q_e\cdot\mathbf{q}\cdot(\mathbf{q}\cdot\nabla)\cdot\mathbf{E} + \frac{{q_e}^2}{8\cdot m_e}\cdot(\mathbf{q}\times\mathbf{B})^2} \qquad 45)$$

Magnetic Dipole moment $\quad \mathbf{M} = \frac{-q_e}{2\cdot m_e}\cdot\mathbf{q}\times\mathbf{B} \quad$ due to the magnetic interaction. 46)

Conjugated moment $\quad \mathbf{p} = m_e\cdot\mathbf{q'} + q_e\cdot(\mathbf{q}\times\mathbf{B})$ 47)

Quadrupole term $\quad \frac{1}{2}\cdot q_e\cdot\mathbf{q}\cdot(\mathbf{q}\cdot\nabla)\cdot\mathbf{E}$ 48)

Diamagnetic interaction (quadratic) $\quad \frac{{q_e}^2}{8\cdot m_e}\cdot(\mathbf{q}\times\mathbf{B})^2$ 49)

The term $-\mu\cdot\mathbf{E_T}(\mathbf{q},t) - \mathbf{M}\cdot\mathbf{B}$, considering the maximum values, I find: $\left|\mu\cdot\mathbf{E_T}\right| = q_e\cdot|\mathbf{q}|\cdot\left|\mathbf{E_T}\right|$,

$$|\mathbf{M}\cdot\mathbf{B}| = \frac{q_e}{2\cdot m}\cdot|\mathbf{r}|\cdot m\cdot|\mathbf{r'}|\cdot|\mathbf{B}| = \frac{q_e}{2}\cdot|\mathbf{r}|\cdot|\mathbf{r'}|\cdot|\mathbf{B}|.$$

Furthermore $\quad \frac{|\mathbf{M}\cdot\mathbf{B}|}{\left|\mu\cdot\mathbf{E_T}\right|} = \frac{\left(\frac{q_e}{2}\cdot|\mathbf{q}|\cdot|\mathbf{q'}|\cdot|\mathbf{B}|\right)}{\left(q_e\cdot|\mathbf{q}|\cdot\left|\mathbf{E_T}\right|\right)} = \frac{|\mathbf{q'}|}{2}\cdot\frac{|\mathbf{B}|}{\left|\mathbf{E_T}\right|} = \frac{|\mathbf{q'}|}{2}\cdot\frac{\eta}{c}$, but $|\mathbf{q'}| \ll \left(\frac{c}{\eta}\right) \Rightarrow \left[\left(\frac{\eta\cdot|\mathbf{q'}|}{c}\right) \ll 1\right]$, so that:

$$\left|\mathbf{M}\cdot\mathbf{B}\right| \ll \left|\mu\cdot\mathbf{E_T}\right|. \qquad 50)$$

Finally I can write the classical Hamiltonian:

$$\mathscr{H} \approx \left(\frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - q_e\cdot V(\mathbf{q}) - \mu\cdot\mathbf{E_T}(\mathbf{q},t)\right)$$

51)

namely, for $\left|\mathbf{q'}\right| \ll \left(\frac{c}{\eta}\right)$ is acceptable the dipole approximation without taking into account of the magnetism.

I look for the corresponding quantum-mechanical Hamiltonian.

QM Hamiltonian operator

Given the classical Hamiltonian $\mathscr{H} = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - q_e\cdot V(\mathbf{q}) - \mu\cdot\mathbf{E_T}(\mathbf{q},t)$ 51')

and the following QM (quantum mechanical) correspondence rules:

Rules 52)

Classical Operator		QM Operator acting on kets or eigenfunctions
$\mathbf{p}$	$\leftrightarrow$	$-j\cdot\hbar\cdot\nabla$
$\mathbf{L}$	$\leftrightarrow$	$-j\cdot\hbar\cdot\mathbf{r}\times\nabla,$
$\mathbf{p}^2$	$\leftrightarrow$	$-\hbar^2\cdot\Delta,$
$\frac{\mathbf{p}\cdot\mathbf{q'}}{2} = \frac{\mathbf{p}^2}{2\cdot m}$	$\leftrightarrow$	$\frac{-\hbar^2}{2\cdot m}\cdot\Delta,$
Energy E	$\leftrightarrow$	$j\cdot\hbar\cdot\frac{\partial}{\partial t},$
$\mathbf{L}^2 = (\mathbf{r}\times\mathbf{p})\cdot(\mathbf{r}\times\mathbf{p}) = r^2\cdot\left(\mathbf{p}^2 - p_r{}^2\right)$	$\leftrightarrow$	$r^2\cdot\left[-\hbar^2\cdot\Delta + \hbar^2\cdot\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\right]$ Sph. coord.
$\mathbf{r}\cdot\mathbf{p}$	$\leftrightarrow$	$-j\cdot\hbar\cdot r\cdot\frac{\partial}{\partial r} = -j\cdot\hbar\cdot r\cdot\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$ Sph. coord.
$\mathbf{A}$ is the vector potential $\mathbf{A}\cdot\mathbf{p}$	$\leftrightarrow$	$\frac{j\cdot\hbar}{2}\cdot(\nabla\bullet\mathbf{A} + \mathbf{A}\cdot\nabla).$

how I get the quantized Hamiltonian? I substitute to each classical operator the one given by the table of the correspondences (at first only the energy E).

Classical mechanical energy $E = T + U = \mathscr{H}$. In QM, E and H are operators acting on a ket: $\mathbf{E} \mid \Psi > = \mathbf{H} \mid \Psi >$

Namely, applying the previous substitutions rules, I get (vectorial operators are written with **bold** fonts):

Classical Hamiltonian	$\leftrightarrow$	QM Hamiltonian
$\boxed{\mathscr{H} = \frac{1}{2}\cdot\mathbf{p}\cdot\mathbf{q'} - q_e\cdot V(\mathbf{q}) - \mu\cdot\mathbf{E_T}(\mathbf{q},t)}$	$\leftrightarrow$	$\boxed{\mathbf{H} = \frac{-\hbar^2}{2\cdot m}\cdot\Delta - q_e\cdot V(\mathbf{q}) - \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)}$

where $\boldsymbol{\mu}$ is the unknown QM linear operator corresponding to the vector dipole moment.

Resulting Hamiltonian operator: $\boxed{\mathbf{H} = \frac{-\hbar^2}{2\cdot m}\cdot\Delta - q_e\cdot V(\mathbf{q}) - \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)}$ 53)

Hamiltonian for macroscopic systems and small interactions close to equilibrium.

I distinguish three partial Hamiltonian:

$$\mathbf{H} = \mathbf{H_0} + \mathbf{H_{int}} + \mathbf{H_r} \qquad 54)$$

Unperturbed Hamiltonian $\mathbf{H_0}$ 55)

Interaction Hamiltonian $\mathbf{H_{int}}$

Relaxation Hamiltonian $\mathbf{H_r}$

Unperturbed Hamiltonian $\mathbf{H_0} = \frac{-\hbar^2}{2\cdot m}\cdot\Delta$ 56)

Interaction Hamiltonian $\mathbf{H_{int}} = \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)$ 57)

Relaxation Hamiltonian $\mathbf{H_r} = q_e\cdot V(\mathbf{q})$ 58)

Finally after a substitution in eq $j\cdot\hbar\cdot\frac{\partial}{\partial t}|\,\Psi > = \mathbf{H}\,|\,\Psi >$, I obtain the ***Schrödinger equation of motion:***

$$\boxed{j\cdot\hbar\cdot\frac{\partial}{\partial t}|\,\Psi_k > = \left(\frac{-\hbar^2}{2\cdot m}\cdot\Delta - q_e\cdot V(\mathbf{q}) - \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)\right)|\,\Psi_k >} \qquad 59)$$

If the system is in a stationary state of energy $E_k = \hbar\cdot\omega_k$, with $|\,\Psi_k(\mathbf{q},t) > = e^{\frac{-j}{\hbar}\cdot E_k\cdot t}\,|\,\psi_k(\mathbf{q}) >$, substituting in the previous equation, I get:

$$\boxed{j\cdot\hbar\cdot\frac{\partial}{\partial t}e^{\frac{-j}{\hbar}\cdot E_k\cdot t}\,|\,\psi_k(\mathbf{q}) > = \left(\frac{-\hbar^2}{2\cdot m}\cdot\Delta - q_e\cdot V(\mathbf{q}) - \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)\right)e^{\frac{-j}{\hbar}\cdot E_k\cdot t}\,|\,\psi_k(\mathbf{q}) >} \qquad 60)$$

On the left side, only the exponential is a function of time, so that the derivative become:

$$\frac{\partial}{\partial t}e^{\frac{-j}{\hbar}\cdot E_k\cdot t}\,|\,\psi_k > = \frac{\partial}{\partial t}e^{\frac{-j}{\hbar}\cdot E_k\cdot t}\,|\,\psi_k > = -\frac{E_k\cdot e^{-\frac{E_k\cdot t\cdot j}{\hbar}}\cdot j}{\hbar}\,|\,\psi_k >$$

which substituted into the equation gives

$$-j\cdot\hbar\cdot\frac{E_k\cdot e^{-\frac{E_k\cdot t\cdot j}{\hbar}}\cdot j}{\hbar}\,|\,\psi_k > = \mathbf{H}\,e^{\frac{-j}{\hbar}\cdot E_k\cdot t}\,|\,\psi_k >$$

resulting, after a simplification, the following time independent eigenvalue equation:

$$\mathbf{H}\,|\,\psi_k(\mathbf{q}) > = E_k\,|\,\psi_k(\mathbf{q}) > \qquad 61)$$

where E_k is the eigenvalue corresponding to the eigenket $|\,\psi_k(\mathbf{q}) >$. The set of all eigenvalues constitutes the discrete spectrum of the operator **H**. The time independent Schrödinger equation now is:

$$\boxed{\left(\frac{-\hbar^2}{2\cdot m}\cdot\Delta - q_e\cdot V(\mathbf{q}) - \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)\right)|\,\psi_k(\mathbf{q}) > = E_k\,|\,\psi_k(\mathbf{q}) >.} \qquad 62)$$

expanding the left side, results $\frac{-\hbar^2}{2\cdot m}\cdot\Delta\,|\,\psi_k > - q_e\cdot V(\mathbf{q})\,|\,\psi_k > - \boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)\,|\,\psi_k > = E\,|\,\psi_k >$

Consider the unperturbed Hamiltonian (in absence of $V(\mathbf{q})$ and $\mathbf{E_T}(\mathbf{q},t)$):

$$\mathbf{H_0}\,|\,\psi_k > = \frac{-\hbar^2}{2\cdot m}\cdot\Delta\,|\,\psi_k > = E_k\,|\,\psi_k >.$$

The Schrödinger equation is: $$\frac{-\hbar^2}{2\cdot m}\cdot\Delta\,|\,\psi_k > = E_k\,|\,\psi_k > \qquad 63)$$

Solution of the one-dimensional Schrödinger equation

Impose the condition that the unperturbed Hamiltonian be ***symmetrical***, (or also ***inversion invariant***) that is:

$$\mathbf{H_0}(p,q) = \mathbf{H_0}(p,-q) \quad \text{symmetry condition} \qquad 64)$$

As a result I can write: $$\mathbf{H_0}(p,q)\,|\,\psi_k(q) > = E_k\,|\,\psi_k(q) > \qquad 65)$$

and also $$\mathbf{H_0}(p,-q)\,|\,\psi_k(-q) > = E_k\,|\,\psi_k(-q) > \qquad 66)$$

and for the hypotheses made $$\mathbf{H_0}(p,q)\,|\,\psi_k(-q) > = E_k\,|\,\psi_k(-q) > \qquad 67)$$

that is possible only if the kets $|\psi_k(q)>$ and $|\psi_k(-q)>$ are eigenfunctions of the same operator corresponding t the same non-degenerated eigenvalue E_k. And therefore the eigenkets $|\psi_k(q)>$ and $|\psi_k(-q)>$ are multiple one of the other. Namely $|\psi_k(-q)> = c_0 |\psi_k(q)>$ where c_0 is a complex constant. As a consequence of that, I have:

$$\mathbf{H_0}(p,q)|\psi_k(q)> = \mathbf{H_0}(p,q)|\psi_k[-(-q)]> = \mathbf{H_0}(p,q)\cdot c_0|\psi_k(-q)> = \mathbf{H_0}(p,q)\cdot c_0^{\,2}|\psi_k(q)> \qquad 68)$$

so that $c_0^{\,2} = \pm 1 \ \Rightarrow |\psi_k(-q)> = \pm|\psi_k(q)>$ therefore the eigenkets are all even (**Even functions: ψ(t)=ψ(-t)**)

or all odd (**Odd functions: ψ(t)=-ψ(-t)**). Namely the eigenkets form ***a finite disparity.***
What are the consequences of the ***finite disparity*** on the interaction Hamiltonian?

Let me consider, therefore, the Interaction Hamiltonian: $\mathbf{H_{int}} = -\boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)$, valid for a single dipole .

For a multitude of dipoles present in the lattice of a crystal, I must address the problem statistically. To do that, I nee the ***matrix elements*** built with the eigenfunctions of the unperturbed symmetrical Hamiltonian and forming *a* ***finite disparity***:

$$\mathbf{H1_{int}}_{i,j} = \left(-<\psi_i|\boldsymbol{\mu}\cdot\mathbf{E_T}(\mathbf{q},t)|\psi_j>\right) \approx \left(-<\psi_i|\boldsymbol{\mu}|\psi_j>\cdot\mathbf{E_T}(\mathbf{q},t)\right) = -\mu_{i,j}\cdot\mathbf{E_T}(\mathbf{q},t) \qquad 69)$$

where the matrix element is:

$$\mu_{i,j} = <\psi_i|\boldsymbol{\mu}|\psi_j> = <\psi_i|\sum_k\left(-q_e\cdot q_k\right)|\psi_j> = -q_e\cdot\sum_k <\psi_i|q_k|\psi_j> \qquad 70)$$

(q_k is the Lagrangian coordinate while q_e is the electron charge)

explicitly: $$\mu_{i,j} = -q_e\cdot\sum_k\left(<\psi_i|q_k|\psi_j>\right) = -q_e\cdot\sum_k\int \overline{\psi_i}\cdot\psi_j\cdot q_k\,dq_k$$

namely: $$\boxed{\mu_{i,j} = -q_e\cdot\sum_k\int \overline{\psi_i}\cdot\psi_j\cdot q_k\,dq_k} \qquad 71)$$

I distinguish two cases:

a) If the eigenkets of the unperturbed Hamiltonian, $\mathbf{H_0}$, are all even (or all odd), it follows that both $|\psi_i>$ and $|\psi_j$

are all even, (or all odd), then the product $\overline{\psi_i}\cdot\psi_j$ is odd and the integral is null, it follows that also $\mu_{i,j} = 0$.

b) If an eigenket is even and the other is odd, then the integrals of the product $\overline{\psi_i}\cdot\psi_j$, are different from zero, and therefore also the corresponding dipolar moment $\mu_{i,j} \neq 0$. It follows that the elements $\mu_{i,i}$ of the main diagonal the matrix, are all zero if the unperturbed Hamiltonian $\mathbf{H_0}$ is *invariant by inversion* or ***symmetrical***. It follows tha using the statistical operator $\boldsymbol{\rho}$, the statistical average of the component α of the dipole moment operator is:

$$<\mu_\alpha> = \mathrm{Tr}(\rho\cdot\mu_\alpha) = \mathrm{Tr}\left[\begin{pmatrix}\rho_{1,1} & \rho_{1,2}\\ \rho_{2,1} & \rho_{2,2}\end{pmatrix}\cdot\begin{pmatrix}0 & \mu_\alpha\\ \overline{\mu_\alpha} & 0\end{pmatrix}\right] = \mathrm{Tr}\left[\begin{pmatrix}\overline{\mu_\alpha}\cdot\rho_{1,2} & \mu_\alpha\cdot\rho_{1,1}\\ \overline{\mu_\alpha}\cdot\rho_{2,2} & \mu_\alpha\cdot\rho_{2,1}\end{pmatrix}\right] = \overline{\mu_\alpha}\cdot\rho_{1,2} + \mu_\alpha\cdot\rho_{2,1}$$

$$\alpha = x, y, z$$

$$<\mu_x> = \overline{\mu_x}\cdot\rho_{1,2} + \mu_x\cdot\rho_{2,1}$$

$$<\mu_y> = \overline{\mu_y}\cdot\rho_{1,2} + \mu_y\cdot\rho_{2,1}$$

$$<\mu_z> = \overline{\mu_z}\cdot\rho_{1,2} + \mu_z\cdot\rho_{2,1}$$

And will be null also the elements of the main diagonal of the interaction Hamiltonian operator $\mathbf{H1_{int}}_{i,i}$ in matrix form, whose generic element is given by:

$$\mathbf{H1_{int}}_{i,j} = -\mu_{i,j}\cdot\mathbf{E_T}\,. \qquad 72)$$

so I can write $\mathbf{H_0} = \begin{pmatrix}E_1 & 0\\ 0 & E_2\end{pmatrix}$ $\quad \mu_\alpha = \begin{pmatrix}0 & \mu_\alpha\\ \overline{\mu_\alpha} & 0\end{pmatrix}$ $\quad \alpha = x, y, z$ 73)

$$\mu_x = \begin{pmatrix}0 & \mu_x\\ \overline{\mu_x} & 0\end{pmatrix} \qquad \mu_y = \begin{pmatrix}0 & \mu_y\\ \overline{\mu_y} & 0\end{pmatrix} \qquad \mu_z = \begin{pmatrix}0 & \mu_z\\ \overline{\mu_z} & 0\end{pmatrix}$$

Furthermore it results that $\mu_\alpha = \mu_\alpha^\dagger$ Hermitian matrix $\quad \alpha = x, y, z$ 74)

in fact: $$\mu_\alpha^\dagger = \left(\overline{\mu_\alpha}\right)^T = \left[\overline{\begin{pmatrix}0 & \mu_\alpha\\ \overline{\mu_\alpha} & 0\end{pmatrix}}\right]^T = \begin{pmatrix}0 & \overline{\mu_\alpha}\\ \overline{\overline{\mu_\alpha}} & 0\end{pmatrix}^T = \begin{pmatrix}0 & \mu_\alpha\\ \overline{\mu_\alpha} & 0\end{pmatrix} = \mu_\alpha$$

the interaction Hamiltonian operator in matrix form is:

$$\mathbf{H1_{int}} = -\mu\cdot\mathbf{E_T}(\mathbf{q},t) = -\sum_\alpha(\mu_\alpha\cdot E_\alpha) = \sum_\alpha\begin{pmatrix}0 & -\mu_\alpha\cdot E_\alpha\\ -\overline{\mu_\alpha}\cdot E_\alpha & 0\end{pmatrix} \qquad 75)$$

explicitly:

$$\mathbf{H1_{int}} = \begin{pmatrix}0 & -\mu_x\cdot E_x\\ -\overline{\mu_x}\cdot E_x & 0\end{pmatrix} + \begin{pmatrix}0 & -\mu_y\cdot E_y\\ -\overline{\mu_y}\cdot E_y & 0\end{pmatrix} + \begin{pmatrix}0 & -\mu_z\cdot E_z\\ -\overline{\mu_z}\cdot E_z & 0\end{pmatrix}$$

Now I look for the time evolution of the expectation value of the discrete operator dipole moment's α component.

The differential equation that let me study the time evolution of the expectation value of an operator, is the one kno from

QM (eq. (18.1)), that for the vectorial operator dipole moment's α component is:

$$\boxed{\frac{d}{dt}<\mu_\alpha> - <\frac{d}{dt}\mu_\alpha> = \frac{1}{j\cdot\hbar}\cdot\left(<[\,\mu_\alpha,\mathbf{H}\,]>\right)} \qquad 76)$$

Assuming that the dipole moment decrease exponentially with *transversal time constant* *(or damping constant)* T_2

▶ Check the accuracy

the differential equation become: $$\boxed{\frac{d}{dt}<\mu_\alpha> + \frac{<\mu_\alpha>}{T_2} = \frac{1}{j\cdot\hbar}\cdot\left(<[\,\mu_\alpha,\mathbf{H}\,]>\right)} \qquad 77)$$

The Hamiltonian appearing in the commutator of eq 77), is formed by the sum of the unperturbed Hamiltonian and th interaction one:

$$\mathbf{H} = \mathbf{H_0} + \mathbf{H1_{int}} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & 0 \end{pmatrix} = \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix}$$

namely: $$\boxed{\mathbf{H} = \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix}} \qquad 78)$$

Now I can calculate the commutator between the dipole moment's α component operator, and the Hamiltonian preser the right side of 77):

$$[\,\mu_\alpha,\mathbf{H}\,] = \mu_\alpha\cdot\mathbf{H} - \mathbf{H}\cdot\mu_\alpha = \begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix}\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix} - \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix}\cdot\begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix}$$

$\mu_\alpha := \mu_\alpha \qquad E_1 := E_1 \qquad E_2 := E_2 \qquad E_\alpha := E_\alpha$

$$\begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix}\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix} - \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix}\cdot\begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & E_2\cdot\mu_\alpha - E_1\cdot\mu_\alpha \\ E_1\cdot\overline{\mu_\alpha} - E_2\cdot\overline{\mu_\alpha} & 0 \end{pmatrix}$$

that is: $$[\,\mu_\alpha,\mathbf{H}\,] = \begin{bmatrix} 0 & \mu_\alpha\cdot(E_2 - E_1) \\ \overline{-\mu_\alpha}\cdot(E_2 - E_1) & 0 \end{bmatrix}$$

I know that $(E_2 - E_1) = \omega_0\cdot\hbar$ substituting in the previous result, I obtain that the commutator is:

$$[\,\mu_\alpha,\mathbf{H}\,] = \begin{pmatrix} 0 & \mu_\alpha \\ \overline{-\mu_\alpha} & 0 \end{pmatrix}\cdot(E_2 - E_1) = \begin{pmatrix} 0 & \mu_\alpha \\ \overline{-\mu_\alpha} & 0 \end{pmatrix}\cdot\omega_0\cdot\hbar$$

so that, finally, the commutator results to be $[\,\mu_\alpha,\mathbf{H}\,] = \begin{pmatrix} 0 & \mu_\alpha \\ \overline{-\mu_\alpha} & 0 \end{pmatrix}\cdot\omega_0\cdot\hbar = \mu_\alpha\cdot\omega_0\cdot\hbar$

that is $$\boxed{[\,\mu_\alpha,\mathbf{H}\,] = \mu_\alpha\cdot\omega_0\cdot\hbar} \qquad 79)$$

furthermore it is ***anti-Hermitian***, in fact:

$$[\,\mu_\alpha,\mathbf{H}\,] = -\left([\,\mu_\alpha,\mathbf{H}\,]\right)^{\dagger} \qquad \mu_\alpha = \begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix} \qquad 80)$$

Now I substitute 79) in the differential equation of the motion of the average value of the dipole moment's α compon operator 77):

obtaining: $$\boxed{\frac{d}{dt}<\mu_\alpha> + \frac{<\mu_\alpha>}{T_2} = \frac{\omega_0}{j}<\mu_\alpha>} \qquad 81)$$

It is a simple first order differential equation and, collecting $<\mu_\alpha>$, it simplify to:

$$\boxed{\frac{d}{dt}<\mu_\alpha> = -\left(\frac{1}{T_2}-\frac{\omega_0}{j}\right)<\mu_\alpha>}$$

whose solution is: $$<\mu_\alpha> = C_0\cdot e^{-\left(\frac{1}{T_2}+\omega_0\cdot j\right)\cdot t} = C_0\cdot e^{\frac{-t}{T_2}}\cdot e^{-j\cdot\omega_0\cdot t}$$

as was expected.

But, deriving once both sides of 81), with respect to the time, I get

$$\frac{d^2}{dt^2}<\mu_\alpha> + \frac{1}{T_2}\cdot\frac{d}{dt}<\mu_\alpha> = \frac{\omega_0}{j}\frac{d}{dt}<\mu_\alpha> \qquad 82)$$

Let me consider again the equation 76)

$$\boxed{\frac{d}{dt}<\mu_\alpha> - <\frac{d}{dt}\mu_\alpha> = \frac{1}{j\cdot\hbar}\cdot\left(<[\mu_\alpha,\mathbf{H}]>\right)} \qquad 76')$$

the left side is composed by two terms:

1) the average of the time derivative of the operator:

a) $$\boxed{<\frac{d}{dt}\mu_\alpha> = -\frac{<\mu_\alpha>}{T_2}}$$

2) the time derivative of the average of the operator:

$$\frac{d}{dt}<\mathbf{A}> = \frac{1}{j\cdot\hbar}\cdot\left(<[\mathbf{A},\mathbf{H}]>\right) + <\frac{d}{dt}\mathbf{A}>$$

b) $$\frac{d}{dt}<\mu_\alpha> = \frac{1}{j\cdot\hbar}\cdot\left(<[\mu_\alpha,\mathbf{H}]>\right) - \frac{1}{T_2}\cdot\left(<\mu_\alpha>\right)$$

Substituting those results at the right side of eq. 82) I get:

$$\frac{d^2}{dt^2}<\mu_\alpha> + \frac{1}{T_2}\cdot\frac{d}{dt}<\mu_\alpha> = \frac{\omega_0}{j}\left[\frac{1}{j\cdot\hbar}\cdot\left(<[\mu_\alpha,\mathbf{H}]>\right) - \frac{1}{T_2}\cdot\left(<\mu_\alpha>\right)\right] \qquad 83)$$

the average: $<\mu_\alpha>$ on the right side of 83) can be obtained from eq. 81):

$$<\mu_\alpha> = \frac{j}{\omega_0}\cdot\left(\frac{d}{dt}<\mu_\alpha> + \frac{<\mu_\alpha>}{T_2}\right)$$

substituting into eq. 83), I have:

$$\frac{d^2}{dt^2}<\mu_\alpha> + \frac{1}{T_2}\cdot\frac{d}{dt}<\mu_\alpha> = \frac{\omega_0}{j}\left[\begin{array}{l}\frac{1}{j\cdot\hbar}\cdot\left(<[\,\mu_\alpha,\mathbf{H}\,]>\right)\;... \\ +\frac{-1}{T_2}\cdot\frac{j}{\omega_0}\cdot\left(\frac{d}{dt}<\mu_\alpha> + \frac{<\mu_\alpha>}{T_2}\right)\end{array}\right] \qquad 84)$$

Calculation of the expectation value of the commutator: $<[\,\mu_\alpha,\mathbf{H}\,]>$ $\qquad \alpha = x, y, z$

knowing that the Hamiltonian is $\boxed{\mathbf{H} = \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}}$ $\qquad$ 78')

substituting into the commutator I get:

$$[\,\mu_\alpha,\mathbf{H}\,] = [\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix},\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}]$$

calculating the commutator results:

$$[\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix},\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}] = \begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix}\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}\;... \\ +(-1)\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}\cdot\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix}$$

But if I calculate the expectation value of this commutator , I obtain a result different from eq 79) $\omega_0\cdot\hbar\cdot(<\mu_\alpha$
fact I have to consider the difference between averages which is the average of the difference:

$E_1 := E_1 \qquad E_\alpha := E_\alpha \qquad E_2 := E_2 \qquad \mu_\alpha := \mu_\alpha$

$$<[\,\mu_\alpha,\mathbf{H}\,]> = <\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix}\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}> - <\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}\cdot\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix}>$$

After a simplification

$$\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix}\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix} \rightarrow \begin{pmatrix} -E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & E_2\cdot\mu_\alpha \\ -E_1\cdot\overline{\mu_\alpha} & E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{pmatrix}$$

$$\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ -\overline{\mu_\alpha}\cdot E_\alpha & E_2 \end{pmatrix}\cdot\begin{pmatrix} 0 & \mu_\alpha \\ -\overline{\mu_\alpha} & 0 \end{pmatrix} \rightarrow \begin{pmatrix} E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & E_1\cdot\mu_\alpha \\ -E_2\cdot\overline{\mu_\alpha} & -E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{pmatrix}$$

results:

$$<[\,\mu_\alpha,\mathbf{H}\,]> = <\begin{pmatrix} -E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & E_2\cdot\mu_\alpha \\ -E_1\cdot\overline{\mu_\alpha} & E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{pmatrix}> - <\begin{pmatrix} E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & E_1\cdot\mu_\alpha \\ -E_2\cdot\overline{\mu_\alpha} & -E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{pmatrix}>$$

$$<\mathbf{A}> - <\mathbf{B}> = <(\mathbf{A}-\mathbf{B})>$$

$$\begin{pmatrix} -E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & E_2\cdot\mu_\alpha \\ -E_1\cdot\overline{\mu_\alpha} & E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{pmatrix} - \begin{bmatrix} E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & E_1\cdot\mu_\alpha \\ -E_2\cdot\overline{\mu_\alpha} & -(E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}) \end{bmatrix} \text{ simplify } \rightarrow \begin{bmatrix} -2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & -\mu_\alpha\cdot(E_1-E_2) \\ -\overline{\mu_\alpha}\cdot(E_1-E_2) & 2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{bmatrix}$$

the expectation value of the commutator is:

$$<[\,\mu_\alpha,\mathbf{H}\,]> = <\begin{bmatrix} -2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & -\mu_\alpha\cdot(E_1-E_2) \\ -\overline{\mu_\alpha}\cdot(E_1-E_2) & 2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{bmatrix}> \qquad 85)$$

knowing that $\boxed{E_2 - E_1 = \omega_0\cdot\hbar}$

Furthermore I can write the expectation value in a simplified form, as follows:

$$<\begin{bmatrix} -2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} & -\mu_\alpha\cdot(E_1-E_2) \\ -\overline{\mu_\alpha}\cdot(E_1-E_2) & 2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha} \end{bmatrix}> = -2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot\left[<\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}>\right] + \omega_0\cdot\hbar\cdot\left[<\begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix}>\right]$$

First I calculate the expectation value of the Pauli matrix $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$<\sigma_3> = <\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}> = \mathrm{Tr}\left[\rho\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] = \mathrm{Tr}\left[\begin{pmatrix} \rho_{1,1} & \rho_{1,2} \\ \rho_{2,1} & \rho_{2,2} \end{pmatrix}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] = \mathrm{Tr}\left(\begin{pmatrix} \rho_{1,1} & -\rho_{1,2} \\ \rho_{2,1} & -\rho_{2,2} \end{pmatrix}\right) = \rho_{1,1} - \rho_{2,2}$$

$$<\begin{pmatrix} 0 & \mu_\alpha \\ \overline{\mu_\alpha} & 0 \end{pmatrix}> = <\mu_\alpha>$$

finally resulting: $$<[\,\mu_\alpha,\mathbf{H}\,]> = -2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2}) + \omega_0\cdot\hbar\cdot(<\mu_\alpha>) \qquad 86)$$

substituting in eq.:84) I get:

$$\frac{d^2}{dt^2}<\mu_\alpha> + \frac{1}{T_2}\cdot\frac{d}{dt}<\mu_\alpha> = \frac{\omega_0}{j}\left[\frac{1}{j\cdot\hbar}\cdot\left[-2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2}) + \omega_0\cdot\hbar\cdot(<\mu_\alpha>)\right] \ldots \atop + \frac{-1}{T_2}\cdot\frac{j}{\omega_0}\cdot\left(\frac{d}{dt}<\mu_\alpha> + \frac{<\mu_\alpha>}{T_2}\right)\right] \qquad 84')$$

and after a simplification of the right side, I get:

$$\frac{d^2}{dt^2}<\mu_\alpha> + \frac{1}{T_2}\cdot\frac{d}{dt}<\mu_\alpha> = \frac{2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot\omega_0\cdot(\rho_{1,1}-\rho_{2,2})}{\hbar} - \omega_0^{\,2}\cdot(<\mu_\alpha>) - \frac{\frac{d}{dt}<\mu_\alpha>}{T_2} - \frac{<\mu_\alpha>}{T_2^{\,2}}$$

collecting the derivatives at the left side and leaving the constant term at the right side, I find:

$$\boxed{\frac{d^2}{dt^2}<\mu_\alpha> + \frac{2}{T_2}\cdot\frac{d}{dt}<\mu_\alpha> + \left(\omega_0^{\,2} + \frac{1}{T_2^{\,2}}\right)\cdot(<\mu_\alpha>) = \frac{2\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot\omega_0\cdot(\rho_{1,1}-\rho_{2,2})}{\hbar}} \qquad 87)$$

This equation, formally, is like to the equation of a classical harmonic oscillator forced by the electric field E_α .

▸ Solving the equation

This equation can be rewritten as a function of the density operator **ρ**, placing:

$$\rho_{1,1} - \rho_{2,2} = <\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}> = <\mathbf{D}> \qquad 88)$$

Let me consider again the equation of the motion of an operator average **A**:

$$\frac{d}{dt}<\mathbf{A}> - <\frac{\partial}{\partial t}\mathbf{A}> = \frac{1}{j\cdot\hbar}\cdot(<[\,\mathbf{A},\mathbf{H}\,]>)$$

rewritten for the new operator **D**: $$\frac{d}{dt}<\mathbf{D}> - <\frac{\partial}{\partial t}\mathbf{D}> = \frac{1}{j\cdot\hbar}\cdot\left(<[\,\mathbf{D},\mathbf{H}\,]>\right) \qquad 89)$$

place the average derivative $$<\frac{\partial}{\partial t}\mathbf{D}> = -\frac{<\mathbf{D}> - \left(<\mathbf{D}>\right)^{e}}{T_1} \qquad 90)$$

substituting 88) and 90) into 87), results:

$$\frac{d}{dt}<\mathbf{D}> + \frac{<\mathbf{D}> - \left(<\mathbf{D}>\right)^{e}}{T_1} = \frac{1}{j\cdot\hbar}\cdot\left(<[\,\mathbf{D},\mathbf{H}\,]>\right) \qquad 91)$$

The Hamiltonian be: $$\boxed{\mathbf{H} = \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix}} \qquad 78'')$$

it let me calculate the commutator on the right side of 91):

$$[\,\mathbf{D},\mathbf{H}\,] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\cdot\begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix} - \begin{pmatrix} E_1 & -\mu_\alpha\cdot E_\alpha \\ \overline{-\mu_\alpha\cdot E_\alpha} & E_2 \end{pmatrix}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -2\cdot E_\alpha\cdot\mu_\alpha \\ \overline{2\cdot E_\alpha\cdot\mu_\alpha} & 0 \end{pmatrix}$$

resulting: $$[\,\mathbf{D},\mathbf{H}\,] = -2\cdot E_\alpha\cdot\begin{pmatrix} 0 & \mu_\alpha \\ \overline{-\mu_\alpha} & 0 \end{pmatrix} = -2\cdot E_\alpha\cdot\boldsymbol{\mu_\alpha}$$

remember that $$\boldsymbol{\mu_\alpha} = \boldsymbol{\mu_\alpha}^{\dagger} \quad \text{Hermitian matrix} \qquad 74')$$

finally the average is $<[\,\mathbf{D},\mathbf{H}\,]> = -2\cdot E_\alpha\cdot\left(<\boldsymbol{\mu_\alpha}>\right)$ been $<\begin{pmatrix} 0 & \mu_\alpha \\ \overline{-\mu_\alpha} & 0 \end{pmatrix}> = <\boldsymbol{\mu_\alpha}>$

Previously I found that eq 81): $$\boxed{\frac{d}{dt}<\boldsymbol{\mu_\alpha}> + \frac{<\boldsymbol{\mu_\alpha}>}{T_2} = \frac{\omega_0\cdot\hbar}{j\cdot\hbar}<\boldsymbol{\mu_\alpha}>} \qquad 81')$$

from which I have $$\frac{1}{j\cdot\hbar}<\boldsymbol{\mu_\alpha}> = \frac{1}{\omega_0\cdot\hbar}\cdot\left(\frac{d}{dt}<\boldsymbol{\mu_\alpha}> + \frac{<\boldsymbol{\mu_\alpha}>}{T_2}\right)$$

$$\omega_0 = \frac{E_2 - E_1}{\hbar}$$

After a substitution in eq. 89), I find that:

$$\frac{d}{dt}<\mathbf{D}> + \frac{<\mathbf{D}> - \left(<\mathbf{D}>\right)^{e}}{T_1} = \frac{-2\cdot E_\alpha}{j\cdot\hbar}\cdot\left(<\boldsymbol{\mu_\alpha}>\right) = \frac{-2\cdot E_\alpha}{\omega_0\cdot\hbar}\cdot\left(\frac{d}{dt}<\boldsymbol{\mu_\alpha}> + \frac{<\boldsymbol{\mu_\alpha}>}{T_2}\right)$$

that is: $$\frac{d}{dt}<\mathbf{D}> + \frac{<\mathbf{D}> - \left(<\mathbf{D}>\right)^{e}}{T_1} = \frac{-2\cdot E_\alpha}{\omega_0\cdot\hbar}\cdot\left(\frac{d}{dt}<\boldsymbol{\mu_\alpha}> + \frac{<\boldsymbol{\mu_\alpha}>}{T_2}\right) \qquad 92)$$

Equilibrium density operator: $\left(<\mathbf{D}>\right)^{e} = \left(\rho_{1,1} - \rho_{2,2}\right)_{e}$ $\qquad <\mathbf{D}> = \rho_{1,1} - \rho_{2,2}$

substituting in eq. 90), it assumes the form:

$$\frac{d}{dt}(\rho_{1,1}-\rho_{2,2})+\frac{\rho_{1,1}-\rho_{2,2}-(\rho_{1,1}-\rho_{2,2})_e}{T_1}=\frac{-2\cdot E_\alpha}{\hbar\cdot\omega_0}\cdot\left[\frac{d}{dt}<\mu_\alpha>+\frac{1}{T_2}\cdot(<\mu_\alpha>)\right] \quad 93)$$

Now, I will describe the time evolution of the ***polarization*** per unit of crystal volume (M_{ar} states for arithmetic average) where are present N_p dipoles.

The polarization is:

$$\mathbf{P}_\alpha=\frac{\sum_{i=1}^{N_p}(<\mu_\alpha>)_i}{V}=\frac{N_p}{V}\cdot\frac{\sum_{i=1}^{N_p}(<\mu_\alpha>)_i}{N_p}=N_V\cdot M_{ar}(<\mu_\alpha>)$$

$$\boxed{\mathbf{P}_\alpha=N_V\cdot M_{ar}(<\mu_\alpha>)} \qquad m^{-3}\cdot C\cdot m=\frac{C}{m^2} \quad 94)$$

Spatial dipolar moment average value $M_{ar}(<\mu_\alpha>)=\frac{\sum_{i=1}^{N_p}(<\mu_\alpha>)_i}{N}$ 95)

Active centers (or polarized molecules) density: $N_V=\frac{N_p}{V}$. 96)

Now I will try to modify eq. 87) at the light of the previous definition (94), 95), 96)). I rewrite eq. 87):

$$\boxed{\frac{d^2}{dt^2}<\mu_\alpha>+\frac{2}{T_2}\cdot\frac{d}{dt}<\mu_\alpha>+(<\mu_\alpha>)\cdot\left(\omega_0^{\,2}+\frac{1}{T_2^{\,2}}\right)=\frac{-2\cdot\omega_0\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})}{\hbar}} \quad 87')$$

Multiply both sides of eq. 87) by N_V :

$$\boxed{\begin{aligned}&\frac{d^2}{dt^2}\left[N_V\cdot(<\mu_\alpha>)\right]+\frac{2}{T_2}\cdot\frac{d}{dt}\left[N_V\cdot(<\mu_\alpha>)\right]\ \ldots=\frac{-2\cdot N_V\cdot\omega_0\cdot E_\alpha\cdot\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})}{\hbar}\\&+N_V\cdot(<\mu_\alpha>)\cdot\left(\omega_0^{\,2}+\frac{1}{T_2^{\,2}}\right)\end{aligned}} \quad 98)$$

then I calculate a spatial average of both sides:

$$\boxed{\begin{array}{l}\left[\frac{\partial^2}{\partial t^2}\left[N_V\cdot\frac{\sum_{i=1}^{N_p}\left(<\mu_\alpha>\right)_i}{V}\right]\right]\ldots \qquad = \frac{-2\cdot N_V\cdot\omega_0\cdot E_\alpha}{\hbar}\cdot\frac{\sum_{i=1}^{N_p}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right]_i}{V}\\ +\frac{2}{T_2}\cdot\frac{\partial}{\partial t}\left[N_V\cdot\frac{\sum_{i=1}^{N_p}\left(<\mu_\alpha>\right)_i}{V}\right]\ldots\\ +N_V\cdot\left[\frac{\sum_{i=1}^{N_p}\left(<\mu_\alpha>\right)_i}{V}\right]\cdot\left(\omega_0^{\,2}+\frac{1}{T_2^{\,2}}\right)\end{array}}$$

as previously defined $\frac{\sum_{i=1}^{N_p}\left(<\mu_\alpha>\right)_i}{N} = M_{ar}\left(<\mu_\alpha>\right)$ which substituted into the equation gives

$$\boxed{\begin{array}{l}\frac{\partial^2}{\partial t^2}\left(N_V\cdot M_{ar}\left(<\mu_\alpha>\right)\right)+\frac{2}{T_2}\cdot\frac{\partial}{\partial t}\left(N_V\cdot M_{ar}\left(<\mu_\alpha>\right)\right)\ldots = \frac{-2\cdot N_V\cdot\omega_0\cdot E_\alpha\cdot M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right]}{\hbar}\\ +N_V\cdot M_{ar}\left(<\mu_\alpha>\right)\cdot\left(\omega_0^{\,2}+\frac{1}{T_2^{\,2}}\right)\end{array}}$$

The α component of the polarization is: $\boxed{P_\alpha = N_V\cdot M_{ar}\left(<\mu_\alpha>\right)}$ So the equation assumes the simple form:

$$\boxed{\frac{\partial^2}{\partial t^2}P_\alpha+\frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha+P_\alpha\cdot\left(\omega_0^{\,2}+\frac{1}{T_2^{\,2}}\right) = \frac{-2\cdot N_V\cdot\omega_0\cdot E_\alpha\cdot M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right]}{\hbar}} \qquad 99)$$

To a random distribution of the molecules corresponds a random distribution of the components μ_α and $\overline{\mu_\alpha}$, resultin that $\mu_\alpha\cdot\overline{\mu_\alpha}$ and $\rho_{1,1}-\rho_{2,2}$ are uncorrelated, so that I can write:

$$\text{spatial average value: } M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right] = M_{ar}\left(\mu_\alpha\cdot\overline{\mu_\alpha}\right)\cdot M_{ar}(\rho_{1,1}-\rho_{2,2}) \qquad 100)$$

If, instead, the molecules have all the same orientation, then $\mu_\alpha\cdot\overline{\mu_\alpha}$ is statistically independent from $\rho_{1,1}-\rho_{2,2}$, finally resulting:

$$M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right] = \mu_\alpha\cdot\overline{\mu_\alpha}\cdot M_{ar}(\rho_{1,1}-\rho_{2,2}) \qquad 101)$$

Now I consider the case of a low correlation between $\mu_\alpha\cdot\overline{\mu_\alpha}$ and $\rho_{1,1}-\rho_{2,2}$ namely:

$$\text{spatial average value: } M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right] = M_{ar}\left(\mu_\alpha\cdot\overline{\mu_\alpha}\right)\cdot M_{ar}(\rho_{1,1}-\rho_{2,2}). \qquad 100")$$

Than I can write:

$$M_{ar}\left[N_V\cdot(\rho_{1,1}-\rho_{2,2})\right] = M_{ar}(N_V\cdot\rho_{1,1})-M_{ar}(N_V\cdot\rho_{2,2}) = N_V\cdot\left(M_{ar}(\rho_{1,1})-M_{ar}(\rho_{2,2})\right)$$

$$N_V = \frac{N_p}{V} \quad M_{ar}\left[N_V\cdot(\rho_{1,1}-\rho_{2,2})\right] = \frac{N_p}{V}\cdot\left(M_{ar}(\rho_{1,1})-M_{ar}(\rho_{2,2})\right) = \frac{N_p}{V}\cdot\left[\frac{\sum_j(\rho_{1,1})_j}{N_p}\right]-\frac{N_p}{V}\cdot\left[\frac{\sum_j(\rho_{2,2})_j}{N_p}\right]$$

$$M_{ar}\left[N_V\cdot(\rho_{1,1}-\rho_{2,2})\right] = \frac{\sum_j (\rho_{1,1})_j}{V} - \frac{\sum_j (\rho_{2,2})_j}{V} = N_1 - N_2$$

The spatial average value is $M_{ar}\left[N_V\cdot(\rho_{1,1}-\rho_{2,2})\right] = N_1 - N_2$

and the α component of the polarization is: $\boxed{P_\alpha = N_V\cdot M_{ar}(<\mu_\alpha>) = N_1 - N_2}$ 102)

Molecular density at energetic level 1: $N_1 = \frac{\sum_j (\rho_{1,1})_j}{V}$

Molecular density at energetic level 2: $N_2 = \frac{\sum_j (\rho_{2,2})_j}{V}$

Going back to equation 99) for the polarization operator, below rewritten:

$$\boxed{\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\left(\omega_0^{\,2} + \frac{1}{T_2^{\,2}}\right) = \frac{-2\cdot N_V\cdot\omega_0\cdot E_\alpha\cdot M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right]}{\hbar}} \quad 99')$$

and substituting 102), I obtain the macroscopic equations:

$$N_V\cdot\frac{d}{dt}\left(M_{ar}(\rho_{1,1}-\rho_{2,2})\right)\ ... + \frac{N_V\cdot M_{ar}(\rho_{.1,1}-\rho_{2,2}) - N_V\cdot M_{ar}\left[(\rho_{1,1}-\rho_{2,2})_e\right]}{T_1} = \frac{-2\cdot E_\alpha\cdot N_V}{\hbar\cdot\omega_0}\cdot\left(\frac{\partial}{\partial t}M_{ar}(<\mu_\alpha>) + \frac{1}{T_2}\cdot M_{ar}(<\mu_\alpha>)\right)$$

I define the average value of the transversal field acting on each molecule $E_{\alpha loc} = N_V\cdot E_\alpha$,
the density difference of dipoles is $N_1 - N_2 = N_V\cdot M_{ar}(\rho_{1,1}-\rho_{2,2})$, while
the thermal equilibrium density is $(N_1 - N_2)_e = N_V\cdot M_{ar}\left[(\rho_{1,1}-\rho_{2,2})_e\right]$.
The differential equation 99) simplify to:

$$\boxed{\frac{d}{dt}(N_1 - N_2) + \frac{N_1 - N_2 - (N_1 - N_2)_e}{T_1} = \frac{-2\cdot E_{\alpha loc}}{\hbar\cdot\omega_0}\cdot\left(\frac{\partial}{\partial t}P_\alpha + \frac{1}{T_2}\cdot P_\alpha\right)} \quad 103)$$

Polarization $P_\alpha = N_V\cdot M_{ar}(<\mu_\alpha>)$

$$\boxed{\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\left(\omega_0^{\,2} + \frac{1}{T_2^{\,2}}\right) = \frac{-2\cdot N_V\cdot\omega_0\cdot E_\alpha\cdot M_{ar}\left[\mu_\alpha\cdot\overline{\mu_\alpha}\cdot(\rho_{1,1}-\rho_{2,2})\right]}{\hbar}}$$

The effect of the time harmonic electromagnetic field on the dielectric material is finally described by the two equatic

$$\boxed{\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\left(\omega_0^{\,2} + \frac{1}{T_2^{\,2}}\right) = \frac{-2\cdot\omega_0\cdot E_{\alpha loc}\cdot M_{ar}(\mu_\alpha\cdot\overline{\mu_\alpha})\cdot(N_1 - N_2)}{\hbar}} \quad 104)$$

$$\boxed{\frac{d}{dt}(N_1 - N_2) + \frac{N_1 - N_2 - (N_1 - N_2)_e}{T_1} = \frac{-2\cdot E_{\alpha loc}}{\hbar\cdot\omega_0}\cdot\left(\frac{\partial}{\partial t}P_\alpha + \frac{1}{T_2}\cdot P_\alpha\right)} \quad 105)$$

If results that $(T_2 \cdot \omega_0) \gg 1$ and $(T_1 \cdot \omega_0) \gg 1$ then $\omega_0 \gg \left(\frac{1}{T_2}\right)$ and $\omega_0 \gg \left(\frac{1}{T_1}\right)$ equation 104) simplify to:

$$\boxed{\left(\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\omega_0^2\right) \approx \left[\frac{-2\cdot\omega_0\cdot E_{\alpha loc}\cdot M_{ar}\left(\mu_\alpha\cdot\overline{\mu_\alpha}\right)\cdot(N_1 - N_2)}{\hbar}\right]} \quad 104')$$

Furthermore, considering a time dependence of P_α of the type $P_\alpha(t) = p_\alpha\cdot e^{j\cdot\omega_0\cdot t}$ and $\frac{\partial}{\partial t}P_\alpha = \omega_0\cdot p_\alpha\cdot e^{j\cdot\omega_0\cdot t}\cdot j$

$$\frac{\partial}{\partial t}P_\alpha(t) = \left(\omega_0\cdot p_\alpha\cdot e^{j\cdot\omega_0\cdot t}\cdot j\right) \gg \left(\frac{1}{T_2}\cdot p_\alpha\cdot e^{j\cdot\omega_0\cdot t}\right)$$

$$(\omega_0\cdot p_\alpha) \gg \left(\frac{1}{T_2}\cdot p_\alpha\right)$$

Equation 105) become: $\boxed{\left[\frac{d}{dt}(N_1 - N_2) + \frac{N_1 - N_2 - (N_1 - N_2)_e}{T_1}\right] \approx \left(\frac{-2\cdot E_{\alpha loc}}{\hbar\cdot\omega_0}\cdot\frac{\partial}{\partial t}P_\alpha\right)}$ 105')

Finally the system of equations is:

$$\boxed{\left(\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\omega_0^2\right) \approx \left[\frac{-2\cdot\omega_0\cdot E_{\alpha loc}\cdot M_{ar}\left(\mu_\alpha\cdot\overline{\mu_\alpha}\right)\cdot(N_1 - N_2)}{\hbar}\right]} \quad 106)$$

$$\boxed{\left[\frac{d}{dt}(N_1 - N_2) + \frac{(N_1 - N_2) - (N_1 - N_2)_e}{T_1}\right] \approx \left(\frac{-2\cdot E_{\alpha loc}}{\hbar\cdot\omega_0}\cdot\frac{\partial}{\partial t}P_\alpha\right)} \quad 107)$$

Assume isotropic materials only, then in equation 106), the average $M_{ar}\left(\mu_\alpha\cdot\overline{\mu_\alpha}\right) = M_{ar}\left[\left(\left|\mu_\alpha\right|\right)^2\right]\cdot\delta(\alpha,\alpha)$ (Kronecker δ), moreover, as a further effect of the isotropy, there is the independence of the effects from the directi

that is:

$$M_{ar}\left[\left(\left|\mu_\alpha\right|\right)^2\right] = M_{ar}\left[\left(\left|\mu_x\right|\right)^2\right] = M_{ar}\left[\left(\left|\mu_y\right|\right)^2\right] = M_{ar}\left[\left(\left|\mu_z\right|\right)^2\right]$$

Considering the transition from state 1 to state 2,

$$M_{ar}\left[\left(\left|\mu_{1,2}\right|\right)^2\right] = M_{ar}\left[\left(\left|\mu_1\right|\right)^2\right] + M_{ar}\left[\left(\left|\mu_2\right|\right)^2\right] + M_{ar}\left[\left(\left|\mu_3\right|\right)^2\right] = 3\cdot M_{ar}\left[\left(\left|\mu_\alpha\right|\right)^2\right]$$

$$M_{ar}\left[\left(\left|\mu_\alpha\right|\right)^2\right] = \frac{M_{ar}\left[\left(\left|\mu_{1,2}\right|\right)^2\right]}{3} \quad 108)$$

substituting in eq. 106), I get:

$$\boxed{\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\omega_0^2 = \frac{-2\cdot\omega_0\cdot E_{\alpha loc}\cdot M_{ar}\left[\left(\left|\mu_{1,2}\right|\right)^2\right]\cdot(N_1 - N_2)}{3\cdot\hbar}} \quad 109)$$

The stored energy in a unitary volume is $\boxed{W_{12} = N_1\cdot E_1 + N_2\cdot E_2}$

Adding and subtracting $N_2\cdot\frac{E_1}{2}$ and $N_1\cdot\frac{E_2}{2}$, in the last equation, I find an expression for the stored energy more use

$$W_{12} = N_1\cdot E_1 + N_2\cdot E_2 = \left(\frac{E_1 + E_2}{2}\right)\cdot(N_1 + N_2) + \left(\frac{E_1 - E_2}{2}\right)\cdot(N_1 - N_2)$$

Calculations

keeping in mind tha $N_V = N_1 + N_2$ $\quad \omega_0\cdot\hbar = E_2 - E_1$ $\quad$ the energy $W_{21} = N_1\cdot E_1 + N_2\cdot E_2$ can be rewritten as:

$$N_1 \cdot E_1 + N_2 \cdot E_2 = \left(\frac{E_1 + E_2}{2}\right) \cdot (N_1 + N_2) + \left(\frac{E_1 - E_2}{2}\right) \cdot (N_1 - N_2) = \left(\frac{E_1 + E_2}{2}\right) \cdot N_V - \frac{\omega_0 \cdot \hbar}{2} \cdot (N_1 - N_2)$$

namely $\boxed{W_{12} = N_1 \cdot E_1 + N_2 \cdot E_2 = \left(\frac{E_2 + E_1}{2}\right) \cdot N_V - \frac{\omega_0 \cdot \hbar}{2} \cdot (N_1 - N_2)}$ $\quad \frac{J}{m^3}$ 110)

$$\frac{\partial}{\partial t} W_{12} = -\frac{\omega_0 \cdot \hbar}{2} \cdot \frac{\partial}{\partial t} (N_1 - N_2)$$

I can substitute those results in eq. 107) to obtain a differential equation for the energy.

Consider equation 107) $\boxed{\frac{d}{dt}(N_1 - N_2) + \frac{(N_1 - N_2) - (N_1 - N_2)_e}{T_1} = \frac{-2 \cdot E_{\alpha loc}}{\hbar \cdot \omega_0} \cdot \frac{\partial}{\partial t} P_\alpha}$ 107')

multiply both sides by $\boxed{-\frac{\omega_0 \cdot \hbar}{2}}$

$$\boxed{\frac{d}{dt}\left[-\frac{\omega_0 \cdot \hbar}{2} \cdot (N_1 - N_2)\right] - \frac{\omega_0 \cdot \hbar}{2} \cdot \frac{(N_1 - N_2) - (N_1 - N_2)_e}{T_1} = E_{\alpha loc} \cdot \frac{\partial}{\partial t} P_\alpha} \quad 107'')$$

the terms $-\frac{\omega_0 \cdot \hbar}{2} \cdot (N_1 - N_2) = W_{12} - \left(\frac{E_2 + E_1}{2}\right) \cdot N_V$

and $\frac{\omega_0 \cdot \hbar}{2} \cdot (N_1 - N_2)_e = -W_{12_e} + \left(\frac{E_2 + E_1}{2}\right) \cdot N_V$

substituting in eq 107'') I get:

$$\frac{d}{dt}\left[W_{12} - \left(\frac{E_2 + E_1}{2}\right) \cdot N_V\right] + \frac{W_{12} - \left(\frac{E_2 + E_1}{2}\right) \cdot N_V - W_{12_e} + \left(\frac{E_2 + E_1}{2}\right) \cdot N_V}{T_1} = E_{\alpha loc} \cdot \frac{\partial}{\partial t} P_\alpha \quad 107''')$$

and after a simplification result:

Energy balance equation $\frac{W}{m^3}$ $\quad \boxed{\frac{d}{dt} W_{12} + \frac{W_{12} - W_{12_e}}{T_1} = E_{\alpha loc} \cdot \frac{\partial}{\partial t} P_\alpha}$ $\quad \frac{V}{m} \cdot \frac{C}{m^2 \cdot s} = 1 \cdot \frac{W}{m^3}$ 111)

$E_{\alpha loc} \cdot \frac{\partial}{\partial t} P_\alpha$ is the work per time unite and volume, made by the field on the medium (acting on the polarization), equating the average power density delivered to the medium. (one part of it is dissipated and the other is stored) .

Extract, now, from eq. 110) the difference N_1-N_2 that appears also in eq 109):

I rewrite eq. 110): $\boxed{W_{12} = \left(\frac{E_2 + E_1}{2}\right) \cdot N_V - \frac{\omega_0 \cdot \hbar}{2} \cdot (N_1 - N_2)}$ 110')

resulting: $N_1 - N_2 = \frac{2}{(\omega_0 \cdot \hbar)} \cdot \left[\left(\frac{E_2 + E_1}{2}\right) \cdot N_V - W_{12}\right]$ 112)

rewrite eq 109):

$$\frac{\partial^2}{\partial t^2} P_\alpha + \frac{2}{T_2} \cdot \frac{\partial}{\partial t} P_\alpha + P_\alpha \cdot \omega_0^2 = \frac{-2 \cdot \omega_0 \cdot E_{\alpha loc} \cdot M_{ar}\left[(|\mu_{1,2}|)^2\right] \cdot (N_1 - N_2)}{3 \cdot \hbar}$$

substituting 112) I get the system of differential equations for P_α and W_{12}:

$$\boxed{\frac{\partial^2}{\partial t^2}P_\alpha + \frac{2}{T_2}\cdot\frac{\partial}{\partial t}P_\alpha + P_\alpha\cdot\omega_0{}^2 = \frac{-4\cdot E_{\alpha loc}\cdot M_{ar}\left[\left(\left|\mu_{1,2}\right|\right)^2\right]}{3\cdot\hbar^2}\cdot\left[\left(\frac{E_2+E_1}{2}\right)\cdot N_V - W_{12}\right]} \quad 113)$$

$$\boxed{\frac{d}{dt}W_{12} + \frac{W_{12} - W_{12_e}}{T_1} = E_{\alpha loc}\cdot\frac{\partial}{\partial t}P_\alpha} \quad 114)$$