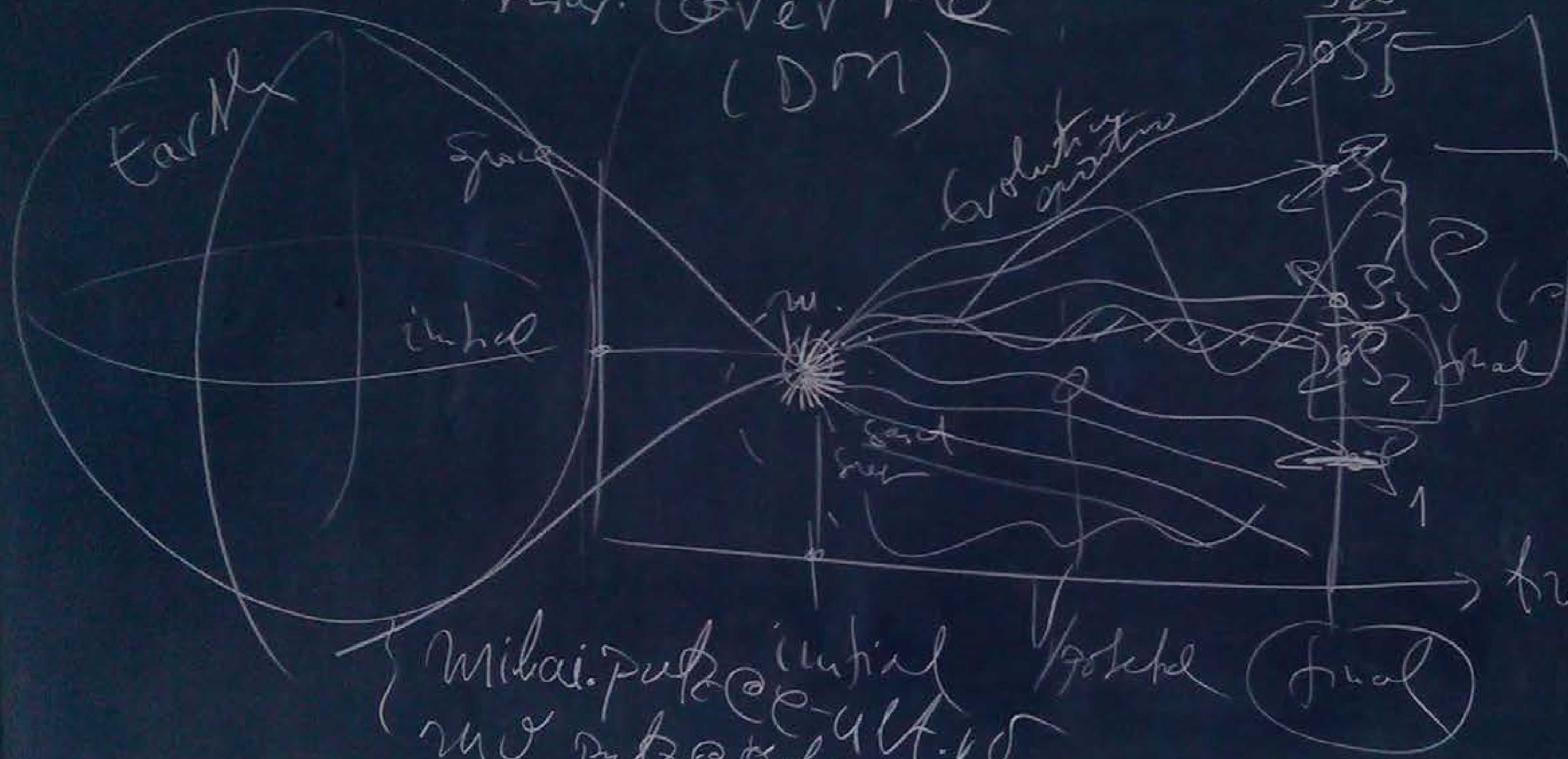


www.miputz.org shown. v0
 ↳ Didactica → Lieke
 ↳ Mky. (over MQ)

Didactica
 Didactice

(over MQ)
 (DM)



ambiguity
 (heterogeneity)

1. Science
2. Simplifying
3. AM in 630
4. Ginkgo tree
5. on HUP
6. Carl Sagan
7. Ginkgo tree

(space) = 7
 coherence
 divergence
 interference
 conflict
 dist. of

mibai.putz@initial
 mibai.putz@e-ult.v0
 mibai.putz@fokers.com

Space Oddity

David Bowie
David Bohm
(Hidden Variables!)

(-∞)
Kruskal
Asymptote

Experimentul cu Două Fante
- La Originea Măsurării Cuantice
- La Originea Moleculară Cuantică

Particle
Arrow

Waves

Wave
Function

(7)

detectors

Heisenberg

So

is the whole

Symmetry
Breakdown
(Uncertainty
Principle)

Hidden
Mystery

White - Black = Grey is the whole
waves - particles as a whole
(Nature of Things)

100
50
25
12.5
6.25
3.125
1.5625
0.78125
0.390625
0.1953125
0.09765625
0.048828125
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Experimentul cu Doua Fonte
 La Originea Mecan. Cuantice
 La Originea Moleculi Cuantice



Paradox $\rightarrow$ 1) Interferența e^- în tunel!

Low's Unoccupied Mol Orbital

2) Divizarea e^- (n-prim unde Hroesou)



Hub-Bond

$1/\sqrt{2}$

$1/\sqrt{2}$

Memoria Def. On the

$1/\sqrt{2}$

$1/\sqrt{2}$



H-Bonding (n-prim unde Hroesou)

Coordination

Quantum Poetry
by M. Cortoese

Quantum Game/Exam

Viata

Puncte - va
sigur o intrare
puncte - va
(un) raspuns!
Fiso cu Molecula

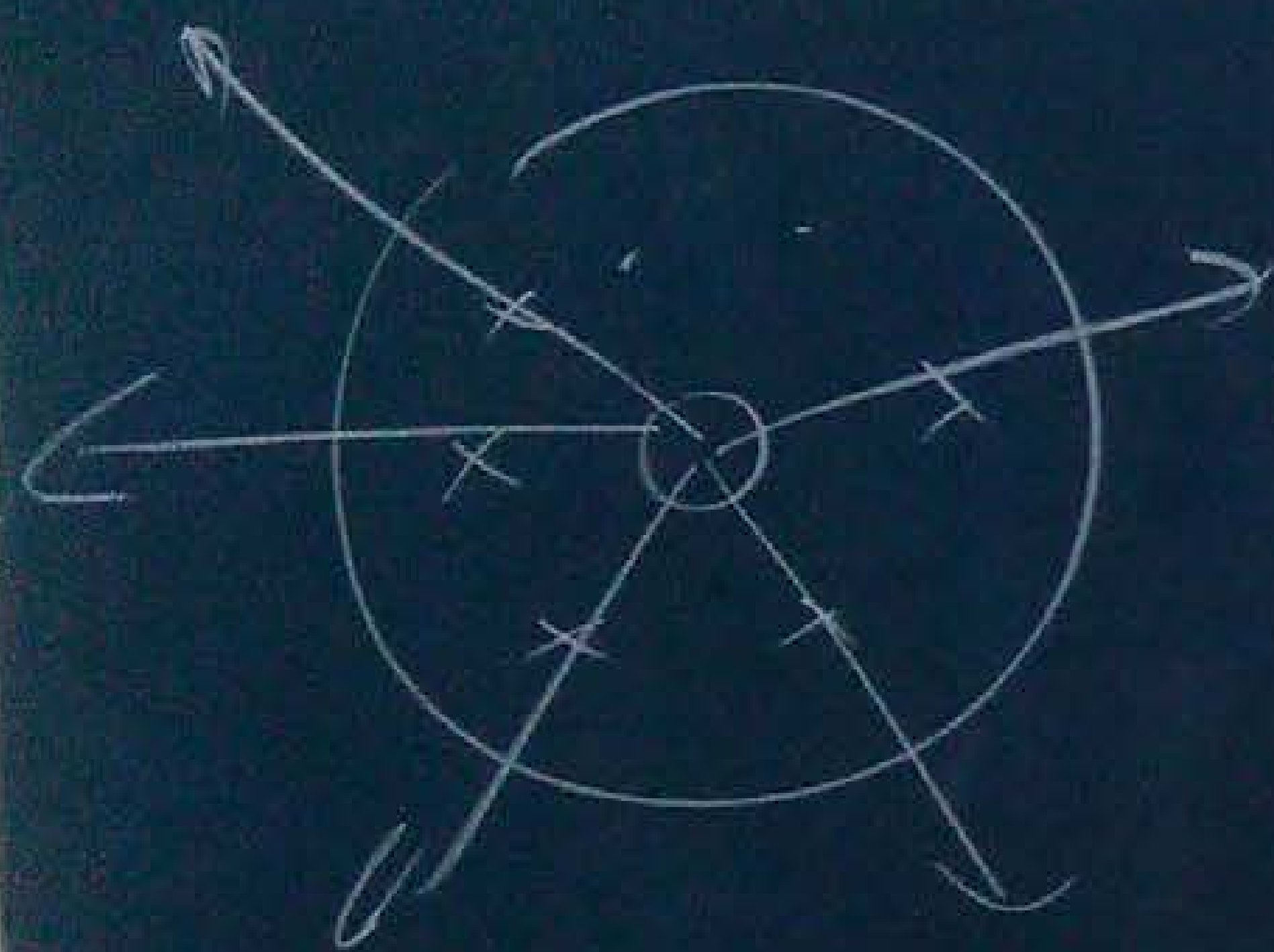
Title (Poetry)
Mile 1st - 2nd
12th - 1st 2nd
1 1/2 5th all around
can fig 2 Bligofe

GAP
TRANSITION
MISSION*

TRAC

Others

Fields



Q-Atom
Quanta-Dots

V
(potential)

Q

Forme

Entanglement
waves

Atom R

Q
Energy

P

~~Total Future~~
~~Future at 100~~
~~Future~~

Doppler effect

Vortices

Filling the whole space
(Ergodicity)

Scattering

Decoherence

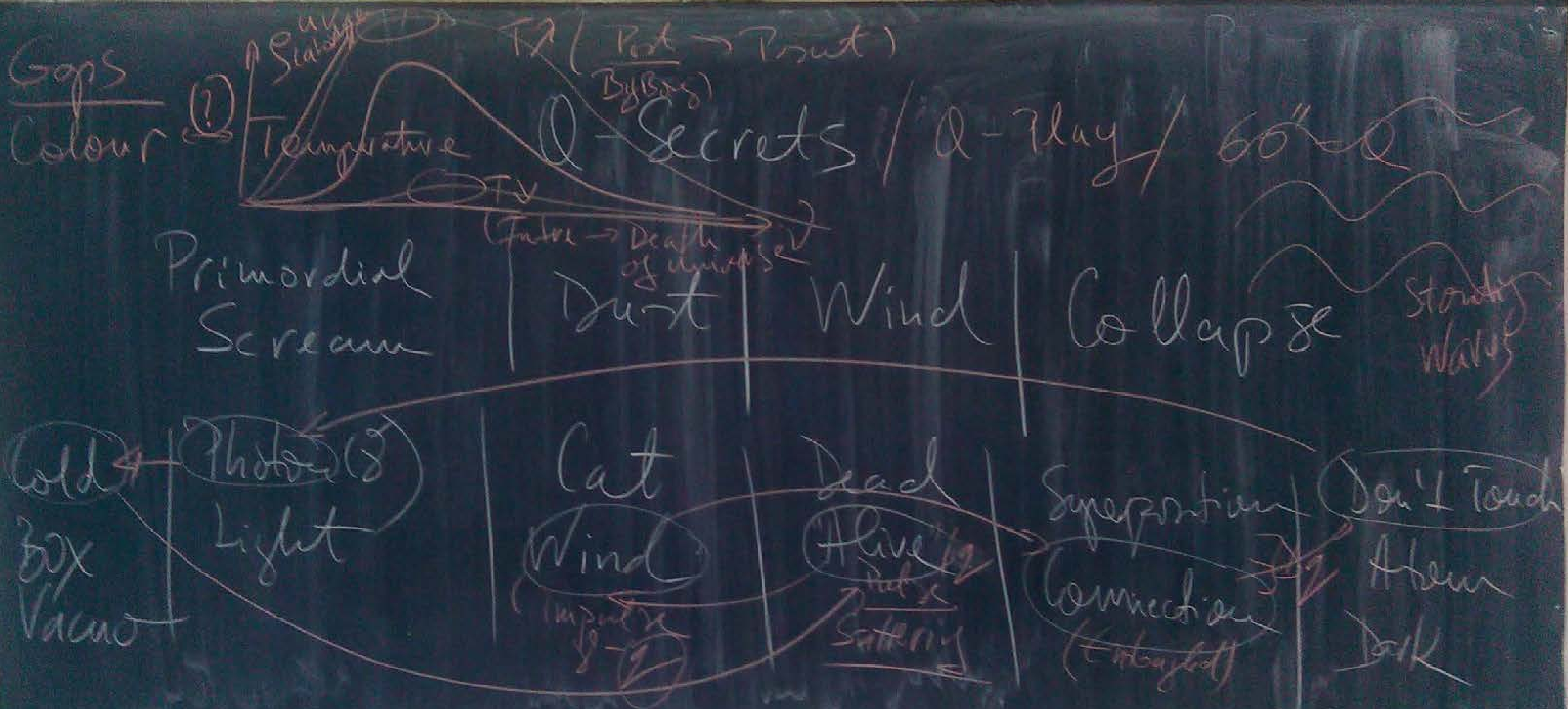
Future

Front

Markov

Port

Collapsing

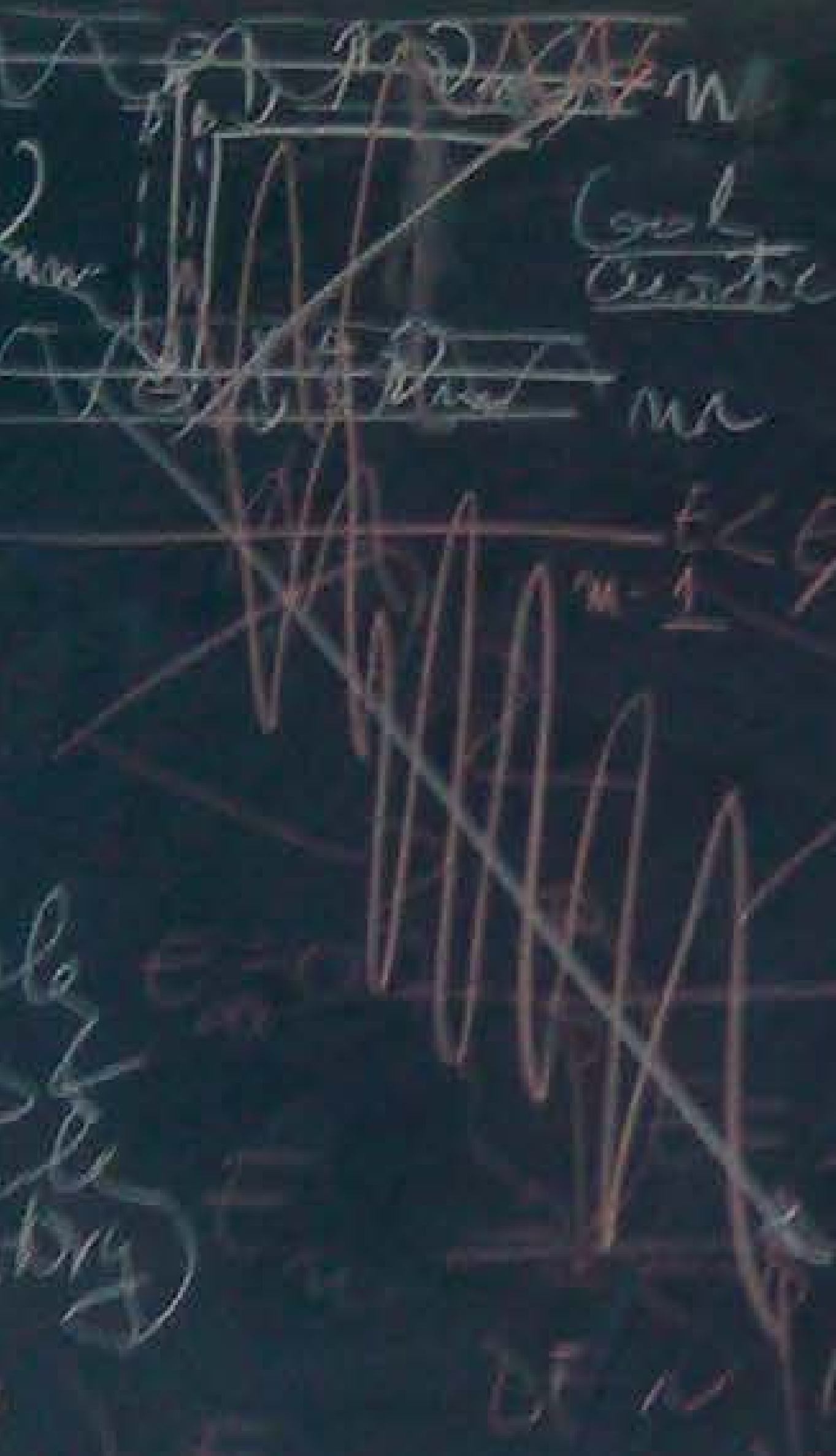


$E = h\nu$
 (Bohr, $n=0$)
 $E = h\nu_m$
 e^-

(Harmon)
 $n = \pm 1/2$

Q-Structure
 of Harmonic
 Oscillator
 (Wigner Solubility)

(1, 1) $E_{1,1}$



Q-Energy

(1/2) Form

Q-Death

Structure

(Harmon)
 Energy

Properties

Golevka
 Structure

→ "The high" (long wave)
 → Under "The high" (long wave)
 (form - long wave)
 → Contribution in structure (under long wave)
 → $2(n) \rightarrow 1(0) \rightarrow 0(0) \rightarrow 0(0)$
 → Under Contribution (under long wave)

Plank

$E = h\nu$

Bohr

$E = h(\nu_0 - \nu_n)$

$$kx' - \omega t' = \frac{\omega}{\sqrt{1-\frac{v^2}{c^2}}} \left(\frac{v}{c^2} x' - t' \right)$$

$$k = \frac{m_0 \gamma v}{\hbar} = \frac{p}{\hbar}$$

$$\Rightarrow p = \hbar k$$

$$= \frac{m_0 c^2}{\hbar \sqrt{1-\frac{v^2}{c^2}}} \left(\frac{v}{c^2} x' - t' \right)$$

Nature

$$p = \frac{h}{\lambda} \text{ (Rel de Broglie)}$$

$$= m_0 \gamma v$$

$$\Rightarrow \omega = \frac{m_0 c^2}{\hbar} = \frac{E_R}{\hbar}$$

$$\Rightarrow E_R = \hbar \omega = E_0$$

Maxima
Power
Fixed
Input

Current
Relativistic

$$E = \hbar \omega = \hbar k v$$

Quantum Statement

Under

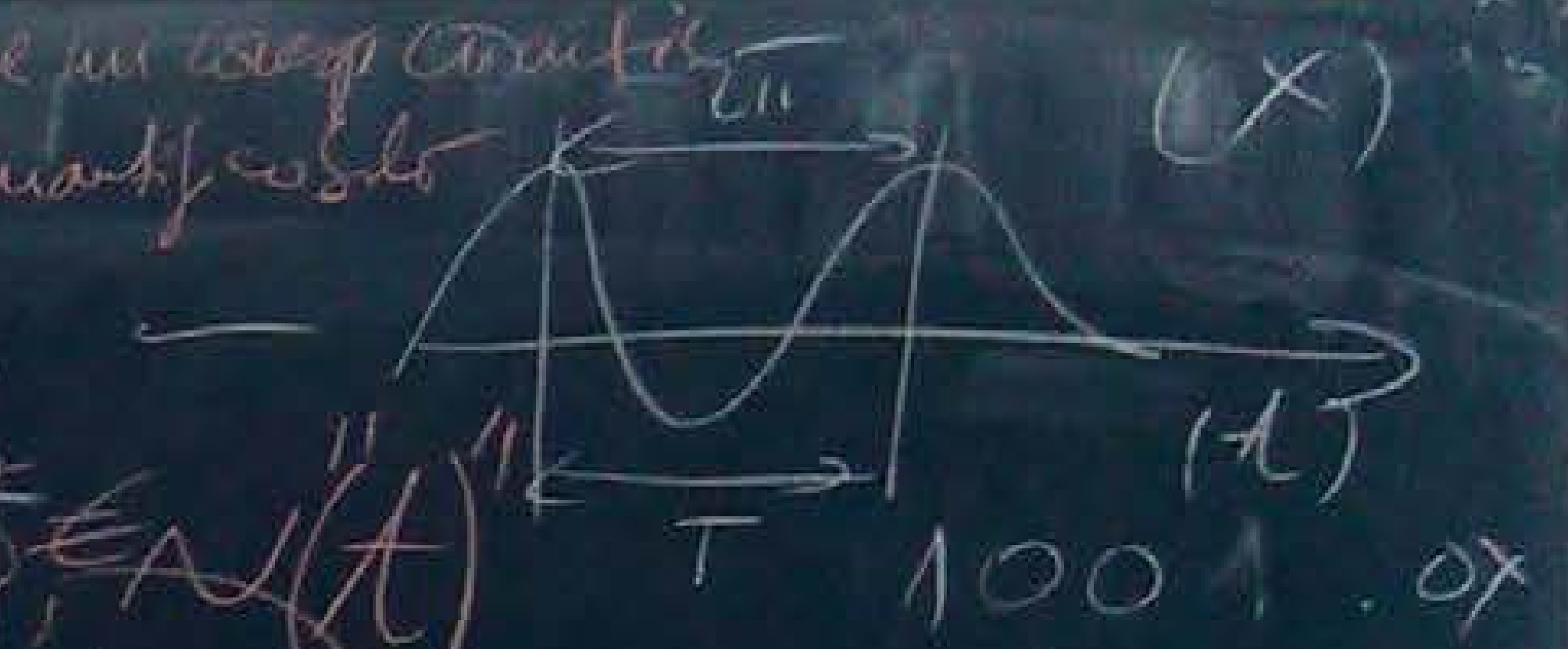
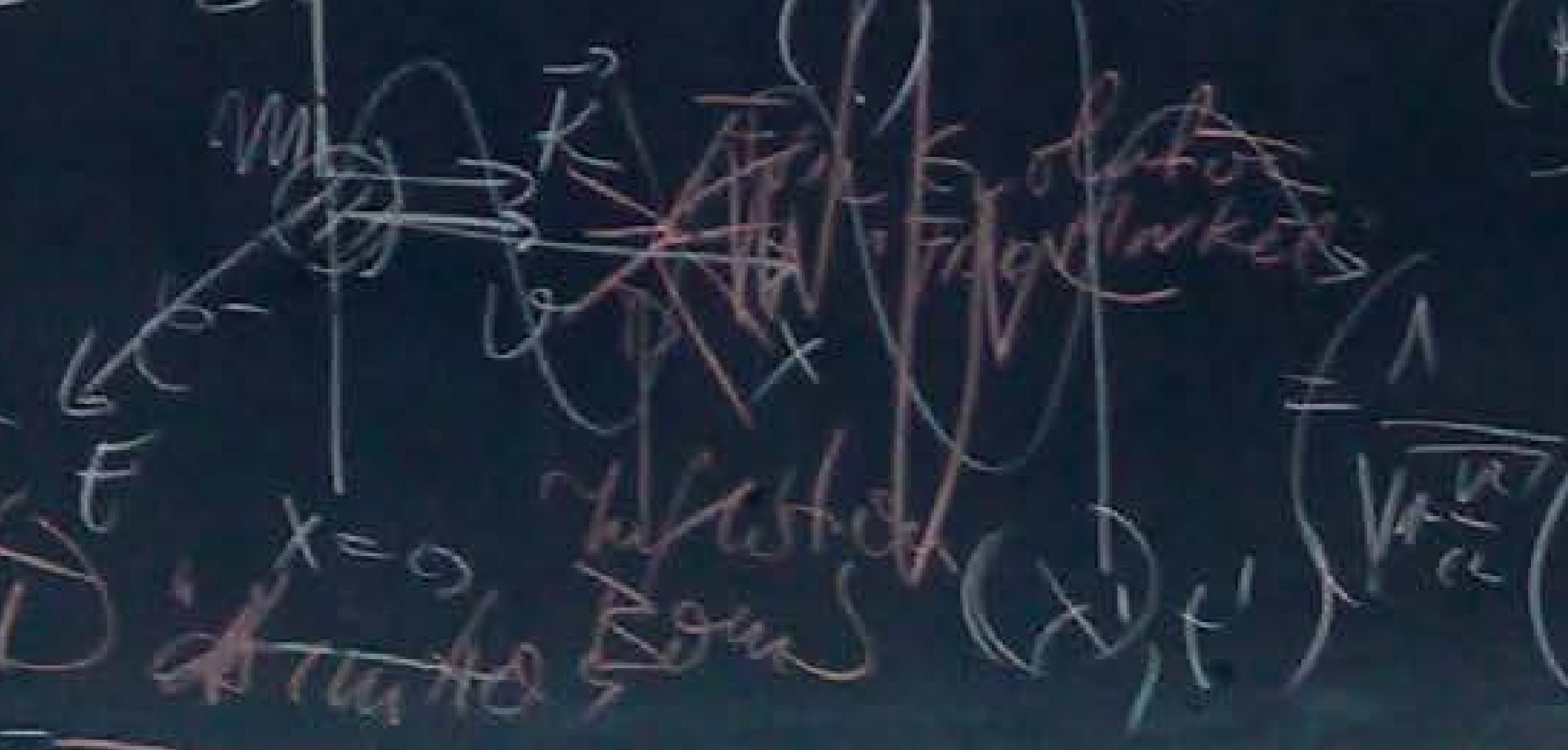
$$E = \hbar \omega = \left(\frac{h}{2\pi} \right) 2\pi \nu = \hbar \omega \Rightarrow \omega = \frac{E}{\hbar}$$

$$\nu = \frac{1}{T}, \lambda, \frac{2\pi}{\lambda} = k$$

Particular

$$E = m_0 c^2$$

$$p = m_0 \gamma v = \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}$$



$$kx - \omega t \sim \frac{2\pi}{\lambda} x - \frac{2\pi}{T} t$$

$$\hbar k = p$$

in evolution

$$kx' - \omega t' = kx - \omega t$$

in Reference

$$t' = \frac{t - \frac{v}{c^2} x}{\sqrt{1-\frac{v^2}{c^2}}}$$

Observability Issue (Problema Observabilității)

Ida Molecule

- Molecule X
- Formula / Structura / Proprietăți
- Name / ACS - American Chemical Society
- (2) Key words + Observability → Science Direct
- (Plt, ppt, doc)

Structure → Proprietăți
"Latente"
("Plus")

Resumat max 1 Pag
(in Bibliografie)

III → Master
→ PhD
→ (81)
Functione
"Nano-Inteligentă"
"Premium / Gold"

Observabilitatea Moleculei X

as a Property

Discrete (Negentropy) Despre Observabilitate (Cuantica)

Universal
S / Dual

hierarchical & integral
(Deformare la mare) (Total Restructur.)

$E \rightarrow At \rightarrow Mol \rightarrow Bio Mol$

+
n
p

General
Information
milieu

Quyroun

Bio-Systeme

Populati

(Indiv. or Atom)

Entropiei
(I)

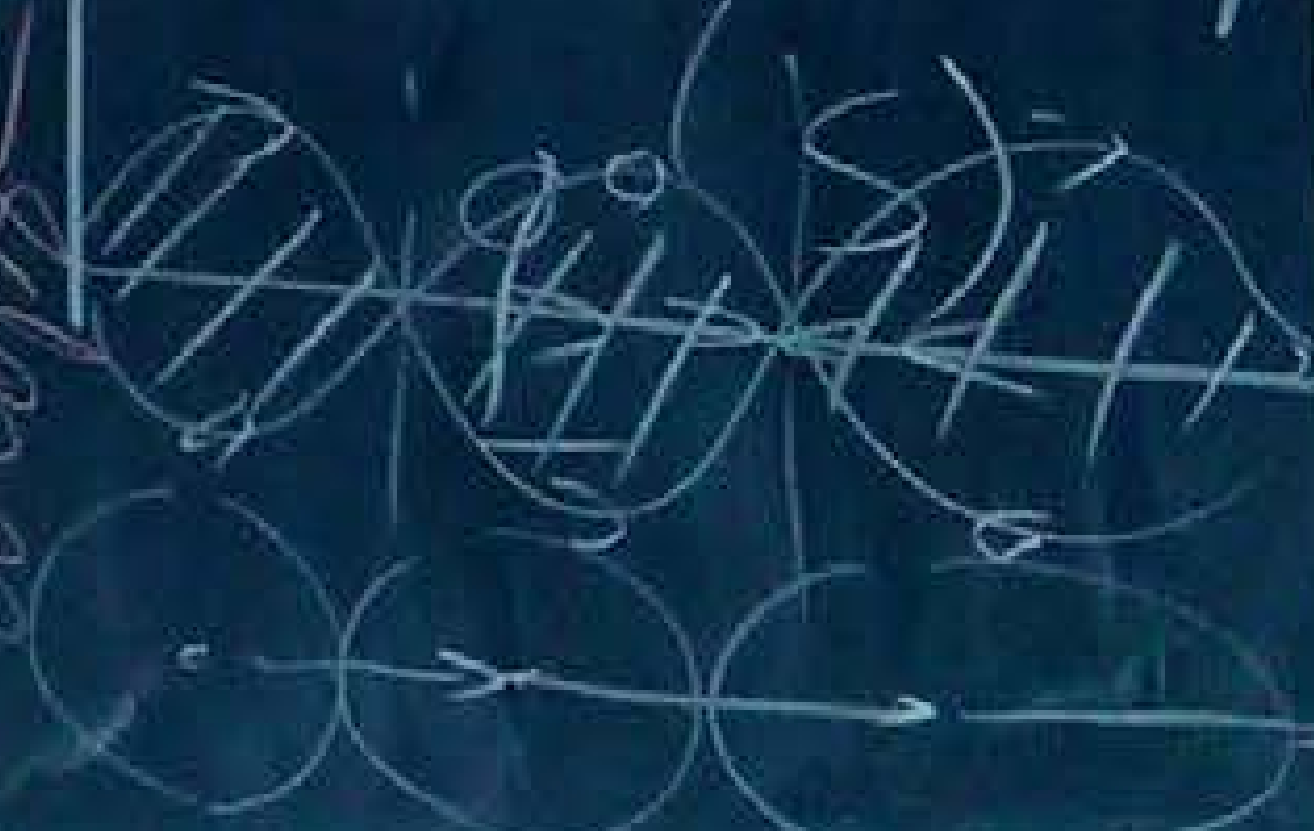
Eufemistic

Evolution
Birth
Death
Loop

Birth
Death
Loop

Death
Decline
Turn of
Involvement

Evolution Entropia / Time



Qualite
Class. $S \rightarrow \infty$
 $I \rightarrow 0$

Universal Dual: $(e^{i\alpha})^2 = 1$

ψ (Wave) $\leftrightarrow$ ψ^* (Conjugate)
 ψ (Wave) $\leftrightarrow$ ψ^* (Conjugate)
 ψ (Wave) $\leftrightarrow$ ψ^* (Conjugate)
 ψ (Wave) $\leftrightarrow$ ψ^* (Conjugate)

Wave & Corpusculi

$\hbar \frac{1}{T} = \hbar \omega$ (Planck)
 $\hbar \frac{1}{\lambda} = \hbar k$ (de Broglie)

$e^{i\alpha} = \cos \alpha + i \sin \alpha$
 $\psi = \frac{1}{\sqrt{2}} (\frac{mv^2}{2}, mc^2, mgh)$

$E = K_B T_{emp}$
 $P_{00} = m_0 \cdot v$
 $\frac{dx}{dt}$

$\Rightarrow \psi = A \cdot e^{\frac{i}{\hbar} (Et - Kx)}$
 uniform wave

integrations: Space-time Continuum

Phase $\phi = \omega t - kx = \frac{E}{\hbar} t - \frac{p}{\hbar} x$
 (invariant) $\psi = A e^{i\phi}$

$\psi(x,t) = |A_{x,t}|^2$

not observable!
 Space interval $\sim \lambda$
 Energy $\sim \hbar \omega$
 Momentum $\sim \hbar k$

OBSERVABILITY

(B) $\varphi \neq ct$ (Transit. wave)

$$\frac{\partial \varphi}{\partial t} = \frac{dx}{dt} = \frac{\partial \omega}{\partial k} \cdot \frac{t}{h} = \frac{dE}{dp}$$

$$E = \sqrt{m_0^2 c^4 + c^2 p^2} = \frac{d}{dp} (m_0^2 c^4 + c^2 p^2) = \frac{1}{2} \frac{2 c^2 p}{\sqrt{m_0^2 c^4 + c^2 p^2}} = \frac{c^2 p}{E} = \frac{c^2 \cdot m v}{m c^2} = v$$

(A) $\frac{\partial \varphi}{\partial t} = \frac{\omega}{h} \cdot \frac{t}{h} = \frac{E}{h} = \frac{m c^2}{h} = \frac{c^2 m_0}{v} > c$

$\varphi = ct(1) \quad dp = 0 = d(\omega t - kx) = \omega dt - k dx$

$$\Rightarrow \frac{dx}{dt} = \frac{\omega}{k}$$

Non-Touch

$$\varphi = (E t - p x) = \omega t - k x$$

Quotient

Classical version

Messung

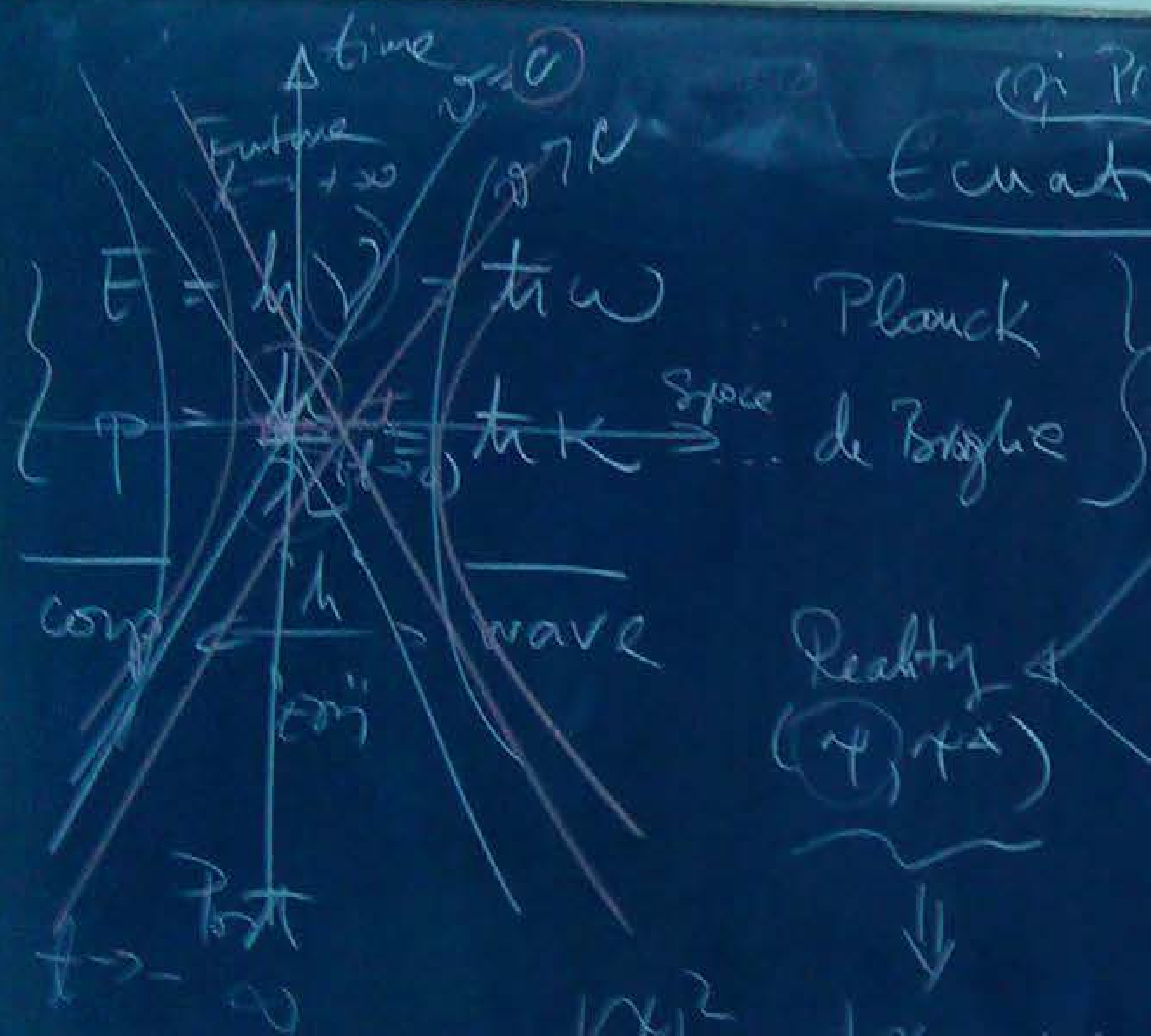
Variable $(x, t) \rightarrow \Delta \varphi \rightarrow \Delta \psi$
(Zeit, dephasing, evolution)

$$\frac{dx}{dt} \quad \text{(Velocity)}$$

Uncertainty
principle I "uncertainty"



(2) Proprietati
Ecuații Cuantice Fundamentale



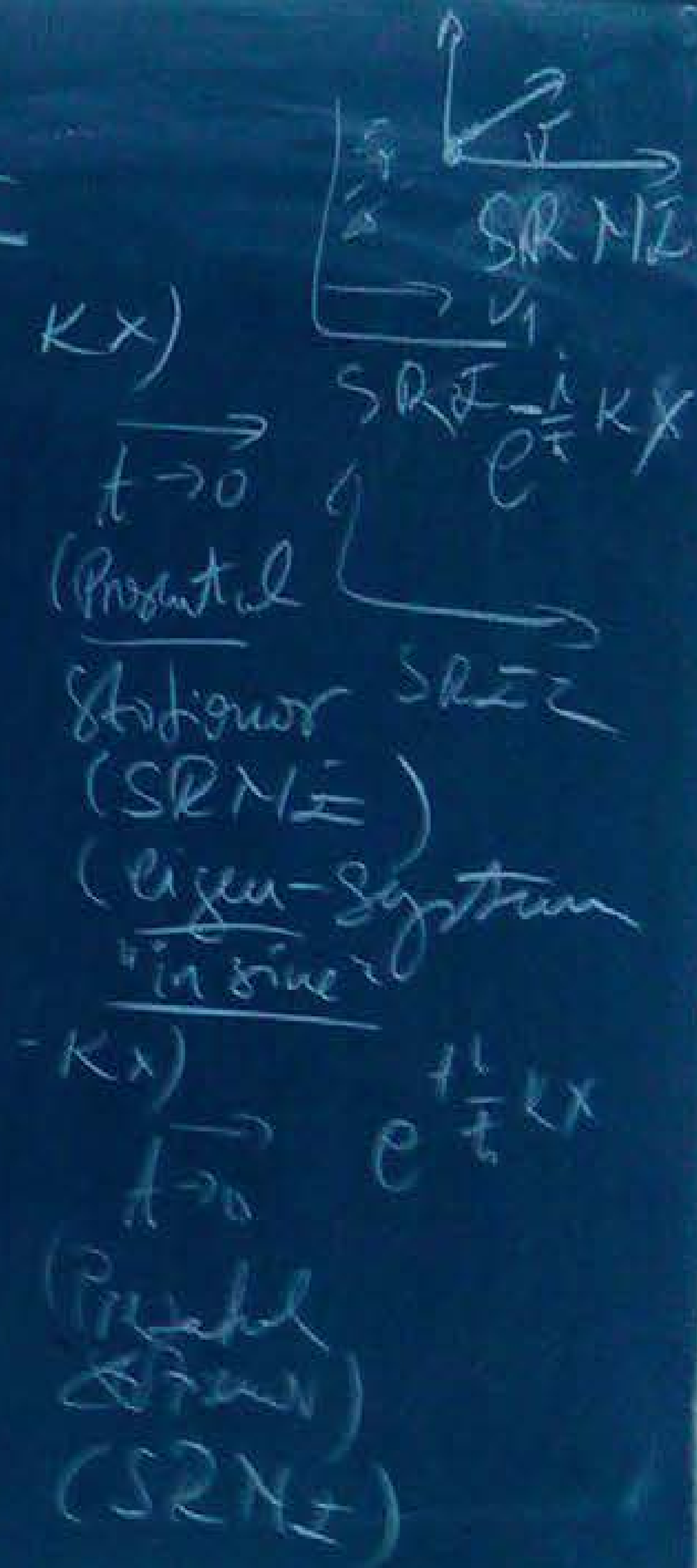
Planck
 de Broglie

Ψ^-
 Hpt. cl.
 (eigen-function)

Reality
 (Ψ, Ψ^*)

$|\Psi|^2 = |\Psi \Psi^*|$ (coupling / collapse)
 (characteristic) → Cu ce probabilitate?

$e^{i \frac{1}{\hbar} (Et - Kx)}$
 'Q'-vibration
 $\Psi^- = e^{-i \frac{1}{\hbar} (Et - Kx)}$



$$\hbar = \frac{h}{2\pi}$$

(di Proprietati) Ecuații Cuantice Fundamentale

$$p = \hbar k$$

$$= \hbar \cdot k = \frac{p}{\hbar}$$

$$\left\{ \begin{array}{l} \psi(x) \approx e^{\frac{i}{\hbar} p x} \\ \psi(p) = \int A(x) e^{\frac{i}{\hbar} p x} dx \end{array} \right. \rightarrow \int \psi(p) e^{\frac{i}{\hbar} p x} dp$$

$$kx = \frac{2\pi}{\lambda} x$$

$$= \left(\frac{2\pi}{\lambda} \right) \frac{\hbar}{\hbar} x$$

$$= k \frac{\hbar}{\hbar} x$$

ψ "eterna"

+ Autoconjugare!

$$1 = \frac{1}{2\pi\hbar} \int dx dp$$

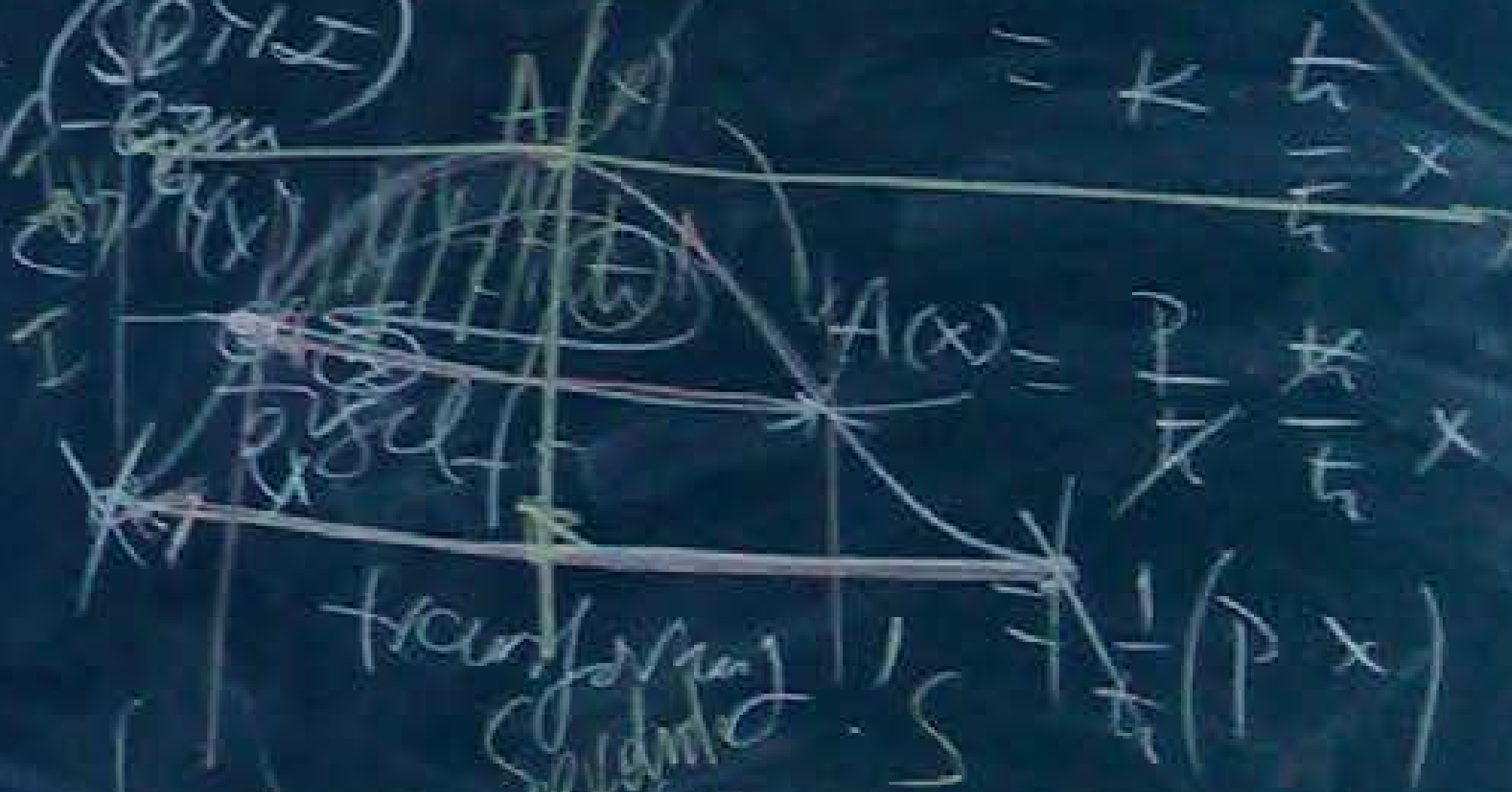
"Unde"
pe un cerc unitate
"2π/ħ"

"transformare" ciclică
în spațiul p

$$\psi(x) = \frac{1}{2\pi\hbar} \int \psi(x) e^{\frac{i}{\hbar} p x} \frac{1}{\hbar} p x$$

$$\Delta x \cdot \Delta p = 2\pi\hbar = h$$

$$\Delta x \Delta p \geq \hbar (2\pi\hbar)$$



$$\psi(x) = \frac{1}{2\pi\hbar} \int \psi(x) dx dp$$

$$\frac{mv^2}{2} = \frac{m^2 v^2 p^2}{2m} \quad (\text{Principiu})$$

Ecuații Cuantice Fundamentale

Ecuația Heisenberg

$$\Delta x \cdot \Delta p = 2\pi \hbar \quad (\text{eg. hipotesa})$$

(ec. de ~~indeterminare~~ cuantice
nedeterminare la observabilitate)

⇒ corol. de nedeterminare
(în cazul inegalităților cuantice)
din exteriorul cilindrului

$$\Delta x \Delta p \geq \hbar$$

Modelul Atomului (Bohr)

$$2\pi r_n \cdot \frac{p_n}{n} = 2\pi \hbar$$

$$r_n p_n = n \hbar$$

ec. cuantice e^- în Atom
(poziția circulară)

$$A = [m=1]$$

$$r_1 p_1 = \hbar$$

$$\Delta x_n = 2\pi r_n$$

$$\Delta p = \frac{p_n}{n}$$

efectul Schrodinger cuantice

Forma funcției
totale
normalizate
(de cunoscut)

$$E = \left(\frac{p^2}{2m} - \frac{Ze^2}{r} \right) = E(n, p)$$

$$\text{Adapt. cuantice} \quad \frac{\partial E}{\partial (p)} = 0 \quad E_0 = \frac{e^2}{4\pi \epsilon_0}$$



Modelul
Bohr
(nu este
un model
real)

temporal $\frac{1}{i} = -i$ $\frac{\partial}{\partial t} \psi(x,t) = \hat{H} \psi(x,t)$ (in Proprietat)

Stationäre $\hat{H} \psi(x) = E \psi(x)$ Equation Quantice Fundamentale

$\psi(x) \cdot = \psi(x) \cdot$
 $\psi(t) \cdot = ?$

$\psi(x,t) = \frac{1}{\sqrt{2}} \left(e^{\frac{i}{\hbar} (px - Et)} \right)$
 (eigen-quantum) $\frac{i}{\hbar} (px - Et)$

$t=0 \rightarrow$ "Stationäre (eigen-stationäre)"
 $x=0 \rightarrow$ "Stationäre (eigen-stationäre)"
 $D \psi \geq 0$ (Rel. Heisenberg'sche Ungleichung)

in die 1. Dimension

$\frac{\partial \psi}{\partial x} = \psi \cdot \frac{i}{\hbar} p \Rightarrow \hat{p}(\psi) = -i\hbar \frac{\partial}{\partial x}(\psi)$
 $\frac{\partial \psi}{\partial t} = \psi \left(-\frac{i}{\hbar} E \right) \Rightarrow \hat{E}(\psi) = i\hbar \frac{\partial}{\partial t}(\psi)$
 $\hat{E}_0 = i\hbar \frac{\partial}{\partial t}$

Ergebnis $\hat{E}_0 = \hat{T}_0 + \hat{V}_0$
 $\hat{E}_0 = \frac{\hat{p}^2}{2m} + \hat{V}(x)$
 (eigen-quantum) $\psi(x,t)$ eq. Schrödinger

$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + V(x) \psi(x,t)$
 $i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x,t)$

Quantum Dialogs

(Dialogues Quantiques)

A ₁		B ₁		A ₂		B ₂		A ₃		B ₃		A ₄		B ₄	
Q ₁	C'est le $\bar{a}$ quant $\bar{a}$		---	Q ₁	C'est le lumina?		---	Q ₁		Qualité de l'onde corpusculaire		Q ₁		Complémentarité l'onde corpusculaire	
Q ₂				Q ₂				Q ₂				Q ₂			
Q ₃				Q ₃				Q ₃				Q ₃			
Q ₄				Q ₄				Q ₄				Q ₄			
Q ₅				Q ₅				Q ₅				Q ₅			
Q ₆				Q ₆				Q ₆				Q ₆			
...				...				...				...			

Proprietăți Cuantice ale Materiei

Se dă

1) SPINUL: eg Schrödinger

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x) \psi$$

Care este spinul electronic?

2) SUPERPOZABILITATE

3) CONTINUITATE

4) OBSERVABILITATE

5) NORMARE

6) ENERGIA OPTIMĂ

(Eiglu - minimă - observabilă)

④ "eiglu" - în siliciu & carbon

⑤ măsurabilitate

② usignu

⑤ probabilitate

$$\frac{\partial}{\partial (tP)} \rightarrow \boxed{P = \frac{1}{2}}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{\hbar^2} \frac{\partial^2 \psi}{\partial t^2}$$

$$S_e = \frac{1}{2}$$

$$S_f = \frac{1}{2}$$

$\bar{e}$ fermion
(eg $\bar{t}$)

γ boson
(eg γ)



Programele Cuantice ale Materiei

Se dă

1) SPINUL : eg Schrödinger

2) SUPERSTABILITATE

3) CONTINUITATE

4) OBSERVABILITATE

5) NORMARE

6) ENERGIA OPTIMĂ

(Eiglu - mărime - observabilă)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x) \psi(t, x)$$

$$\frac{\partial}{\partial (t, x)} \rightarrow \left[\begin{matrix} \frac{1}{2} \\ \frac{1}{2} \end{matrix} \right]$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{\hbar} \frac{\partial}{\partial t} \psi$$

1-Fully, 1/2
teoria
"part-anti-part"

Care este spinul electronic?
 $\hbar \uparrow \leftrightarrow x \uparrow$

$$s_e = \frac{1}{2}$$

$$s_f = \pm 1$$

e^- fermion
(eg $\hbar$)

γ boson
(eg $\hbar$)



Programele Cuantice ale Materiei

- 1) SPINUL
- 2) SUPERDIZABILITATE
- 3) CONTINUITATE
- 4) OBSERVABILITATE
 - ② "eigen"-insiruire cuantice
 - ⑤ măsurabilitate
- 5) NORMARE
 - ② unicuă
 - ⑤ probabilitate
- 6) ENERGIA OPTIMĂ
(eigen-minima-observabilă)

"N"

"UNDA" (de informație)

$$\lim_{x \rightarrow \pm \infty} \psi(x, t) = 0$$

$$\lim_{t \rightarrow \pm \infty} \psi(x, t) = ?$$

$$\lim_{t \rightarrow \pm \infty} \psi(x, t) = ??$$

"Big Bang"

"Big Crash"

"Big Bang"

"Big Bang"

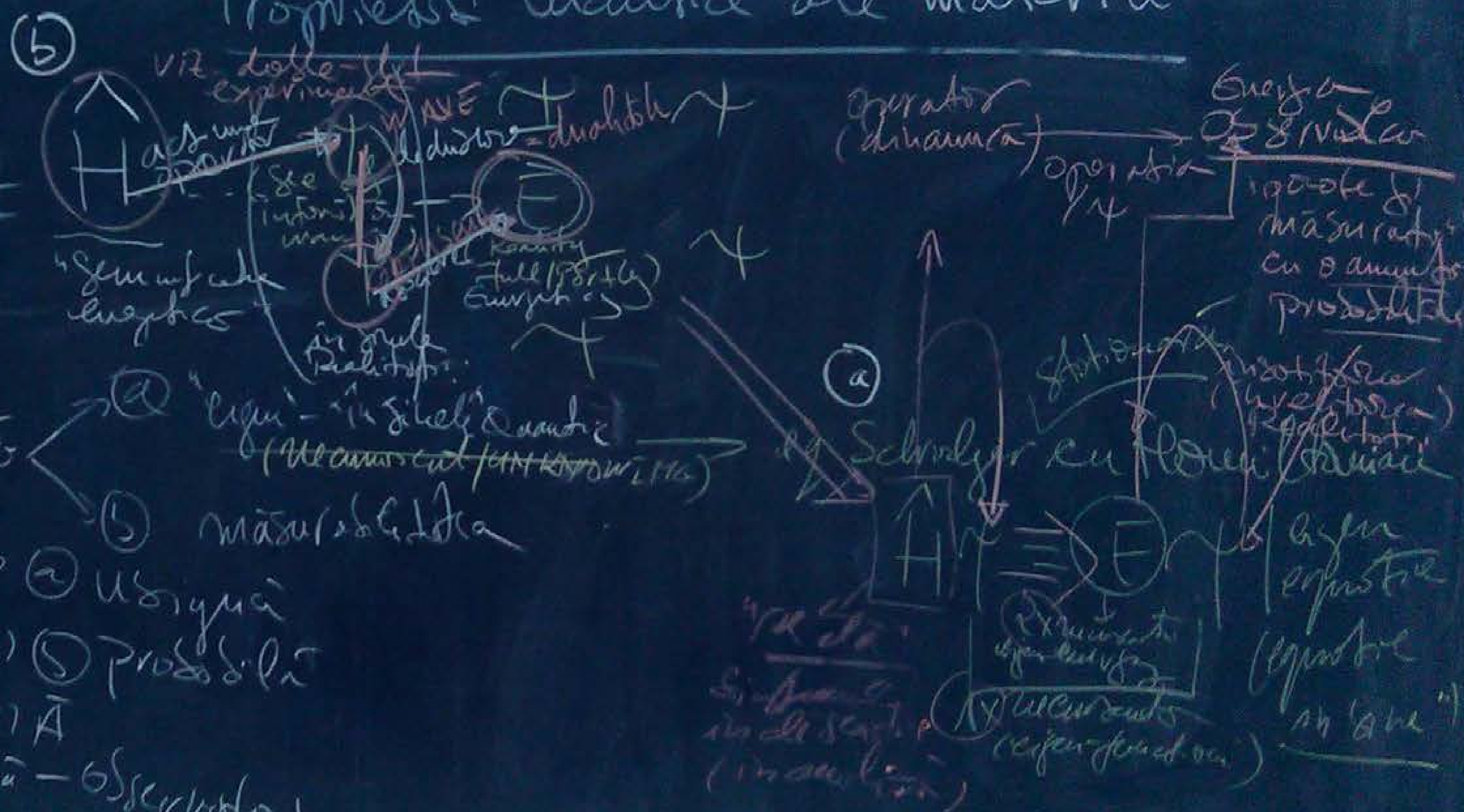
$$\lim_{t \rightarrow \pm \infty} \psi(x, t) = \lim_{t \rightarrow \pm \infty} \psi(x, t)$$

$$\lim_{t \rightarrow \pm \infty} \psi(x, t) = \lim_{t \rightarrow \pm \infty} \psi(x, t)$$

$$\lim_{t \rightarrow \pm \infty} \psi(x, t) = \lim_{t \rightarrow \pm \infty} \psi(x, t)$$



- 1) SPINUL
2) SUPERSTABILITATE
3) CONTINUITATE
4) OBSERVABILITATE
5) NORMARE
6) ENERGIA OPTIMĂ
(Eigen-minimă-observabilă)



Proprietăți Cuantice ale Materiei $\int_{\Gamma} \rho(\psi) d\Gamma \xrightarrow{\Gamma \rightarrow \infty} 1$

1) SPINUL

2) SUPERSTABILITATE

3) CONTINUITATE

4) OBSERVABILITATE

5) NORMARE

6) ENERGIA OPTIMĂ

(Eigen - minimum - operator)

$$\int_{\Gamma} \psi^* \hat{H} \psi d\Gamma = \int_{\Gamma} \psi^* E \psi d\Gamma = E \int_{\Gamma} \psi^* \psi d\Gamma$$

(E constant)

1) Eigen - în starea de echilibriu
(Mechanismul de funcționare)

2) măsurabilitate (E)

3) unicitate

4) probabilitate

$$\hat{H} \psi = E \psi$$

Modelul de funcționare al sistemului de măsurare

Modelul de funcționare al sistemului de măsurare

Modelul de funcționare al sistemului de măsurare

Modelul de funcționare al sistemului de măsurare

Proprietăți Cuantice ale Materiei $\int_{\Gamma} |\psi|^2 d\Gamma \xrightarrow{r \rightarrow \infty} 1$

1) SPINUL

2) SUPERSTABILITATE

3) CONTINUITATE

4) OBSERVABILITATE

5) NORMARE

6) ENERGIA OPTIMĂ
(eigen - minimă - observabilă)

④ "eigen" - în fizică & mecanică
(~~mechanical~~ ~~fundamental~~)

⑤ măsurabilitate (?)

② usor găsită
⑤ probabilă

prin
(continu
minimul
eigen
observabilă)

$$\int_{\Gamma} \psi^* \hat{H} \psi d\Gamma = \int_{\Gamma} \psi^* E \psi d\Gamma = E \int_{\Gamma} \psi^* \psi d\Gamma = E \int_{\Gamma} |\psi|^2 d\Gamma = E$$

(rotor compendiar)

(normalizare)

$$E = \frac{\int_{\Gamma} \psi^* \hat{H} \psi d\Gamma}{\int_{\Gamma} \psi^* \psi d\Gamma}$$

$r \rightarrow \infty$

$$\delta E = 0$$

$$E = \int_{-\infty}^{\infty} \psi^* \hat{H} \psi d\Gamma$$

(observabilă)

DISCONTINUITATE

Progresse Quantice ale Materiei

1) SPINUL

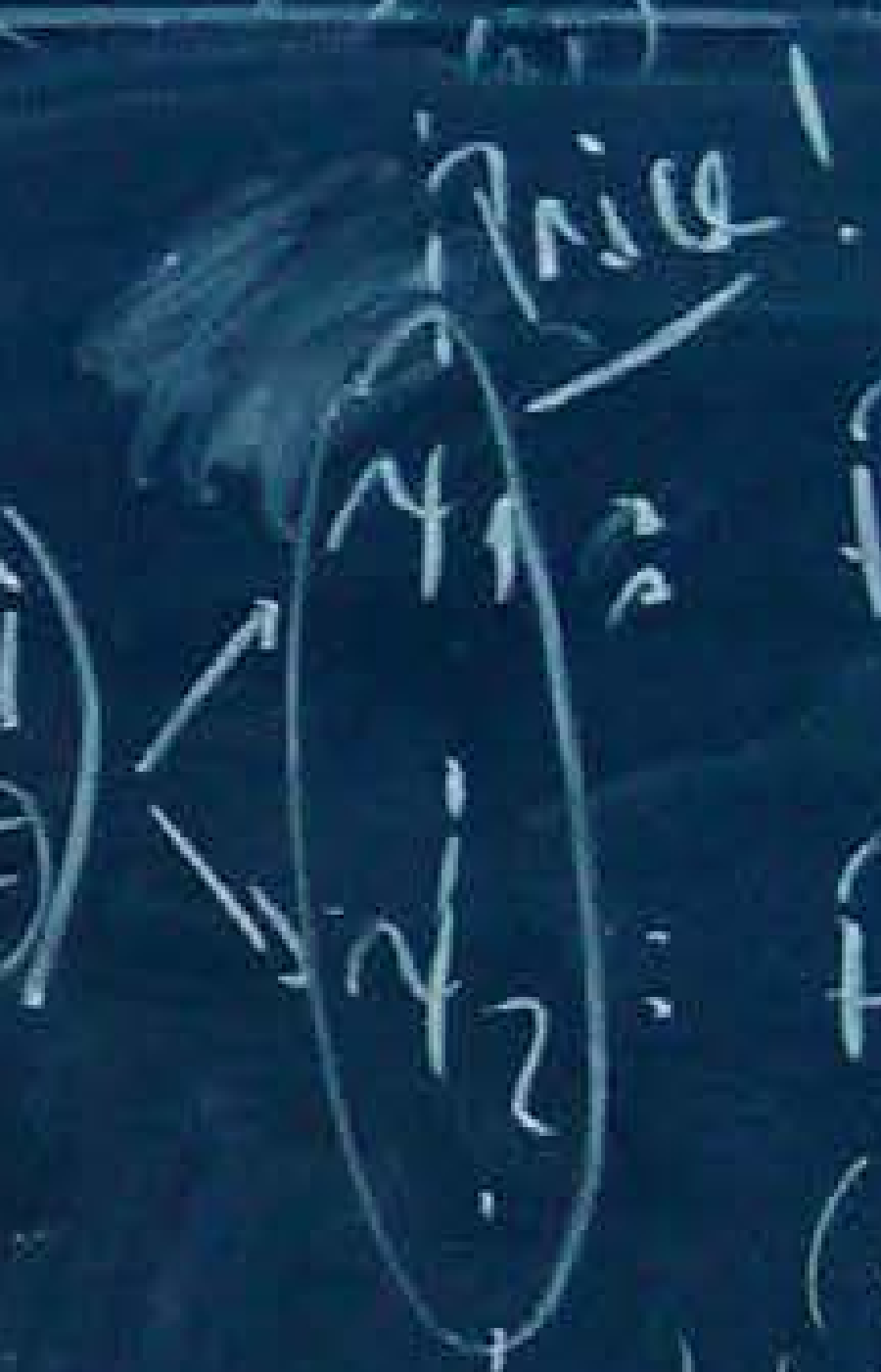
2) SUPERDIZABILITATE $\rightarrow$ viz doble slit

3) CONTINUITATE $\rightarrow$ multiple slits (exp.!!)

4) OBSERVABILITATE $\rightarrow$ a) "eigen" - în starea cuantă
(Measurement / ~~Measurement~~)

5) NORMARE $\rightarrow$ b) măsurabilitate (E)

6) ENERGIA OPTIMĂ
(eigen - minimă - observabilă)



$$\hat{H}\psi_1 = E\psi_1 \text{ (info 1)}$$

$$\hat{H}\psi_2 = E\psi_2 \text{ (info 2)}$$

(Keys of cryptotext)

$$\forall \psi = c_1\psi_1 + c_2\psi_2 \mid \hat{H}\psi = E\psi$$

(all possible info)

$$\hat{H}\psi = \hat{H}(c_1\psi_1 + c_2\psi_2) = c_1\hat{H}\psi_1 + c_2\hat{H}\psi_2 = c_1E\psi_1 + c_2E\psi_2 = E(c_1\psi_1 + c_2\psi_2) = E\psi$$

? E, Ψ | $\hat{H}\Psi = E\Psi$ Vibrația Cuantică Moleculară, Sol. Mole. Bistrița AB

1) ^{Stabiliza} Hamiltonianul
Sistemului în coord.

$\hat{H} = \frac{p^2}{2m_e} + \frac{1}{2} m_e \omega_e^2 x^2$

$+ \frac{1}{2} m_e \omega_e^2 x^2$ ✓
Harmonic

2) Stabiliza Formei
Parametrica a Ψ a
Sist. în coord.

1) Continuă
Derivada
Asimptotică $\rightarrow 0$
 $x \rightarrow \infty$

$\Psi(r_1, r_2) = r_1 e^{-r_2^2 x^2} = \Psi^*(r_1, r_2); r_1, r_2 \in \mathbb{R}$ ✓
 $\frac{1}{N} = \int_{-\infty}^{\infty} \Psi^* \Psi dx = r_1^2 \int_{-\infty}^{\infty} e^{-2r_2^2 x^2} dx = r_1^2 \sqrt{\frac{\pi}{2r_2}}$ ✓

3) Aplicarea condiției
de Normalizare a Ψ
pe tot spațiul de
existență a Sist.

$\int \Psi^* \Psi dr = 1$
 $\Rightarrow$ 0 Relatie între
parametrii Ψ

$E = \int \Psi^* \hat{H} \Psi dx = \frac{r_1^2}{2r_2 m} + \frac{1}{2} \frac{m \omega^2}{r_2^2} = \frac{r_1^2}{2r_2 m} + \frac{1}{2} \frac{m \omega^2}{r_2^2}$ ✓
 $\Rightarrow r_1 = \left(\frac{2r_2}{\pi} \right)^{1/4}$

4) Calculul expresiei
parametrica a energiei

$E = \frac{\int \Psi^* \hat{H} \Psi dr}{\int \Psi^* \Psi dr}$

1) complet
de probabilitate
optim pt
parametrii

$\frac{\partial E}{\partial r_2} = 0 = \frac{r_1^2}{2m} - \frac{1}{2} \frac{m \omega^2}{r_2^3} = \frac{r_1^2}{2m} - \frac{1}{2} \frac{m \omega^2}{r_2^3}$ ✓
 $\Rightarrow r_2 = \frac{m \omega}{2\hbar}$

5) Cond. de optimizare
minimizarea energiei, minimul
a Sist. parametric

$\left(\frac{\partial E}{\partial r_2} \right) = 0$

$E = \frac{1}{2} \hbar \omega$ ✓
Măsurată la (1) ✓
Unimodular
Vibrație cuantică

$$E = \frac{h\omega}{2}$$

$$E = mc^2$$

$$E = h\nu = h\omega$$

$$p = \frac{h}{\lambda}, \quad p = \hbar k$$

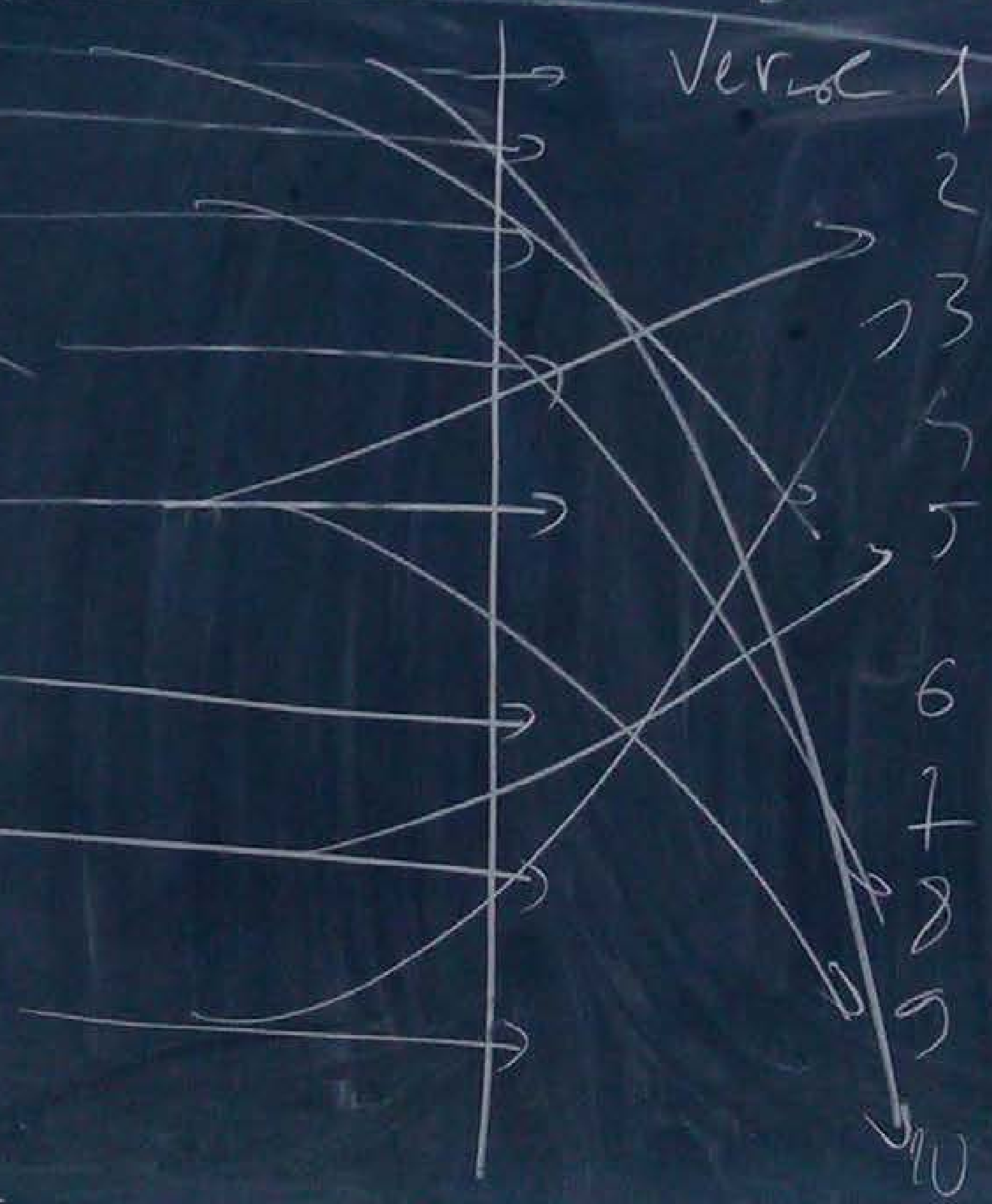
$$\Delta x \cdot \Delta p = \hbar$$

$$\lambda = \frac{1}{k}$$

$$H\psi = E\psi$$

$$H = \frac{\hbar^2 k^2}{2m} + V(x)$$

Quantum Poetry

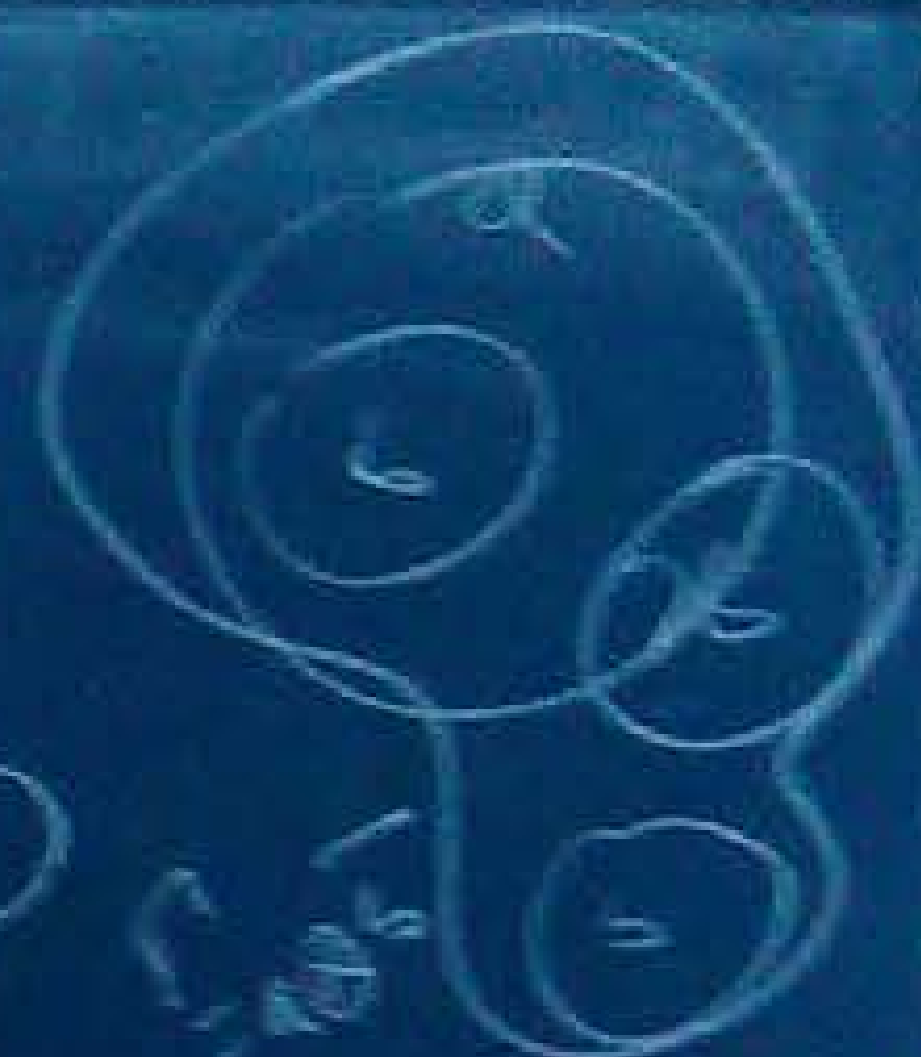


Criptologia Mecanica

In marea etern pulsatorie
Lumina Alargata de drumul
Orbitele nu au somn
Vizata dual
La incertitudinea lumii
Fata - Verso
Vazute si Nevazute
Energia Vietii de Jos!

I Existential Nature - Quantica a Legătorii Chimice

a
5



$$0 = \langle \psi | H | \psi \rangle \Rightarrow \langle \psi | \psi \rangle = 0 \quad | \psi \rangle \neq 0$$

(I) densitat de
potent. $H_{12} = \int \psi_1^* H \psi_2 d\tau$
proba totala. $\int \psi_1^* \psi_1 d\tau = 1$ (autoadjunct)

(II) interactive
 ψ_1, ψ_2
a/b/c
a/b

(no)
observability

$$\langle 0 | 0 \rangle = 1$$

$$A_{12} = \langle \psi_1 | \psi_2 \rangle = 0$$

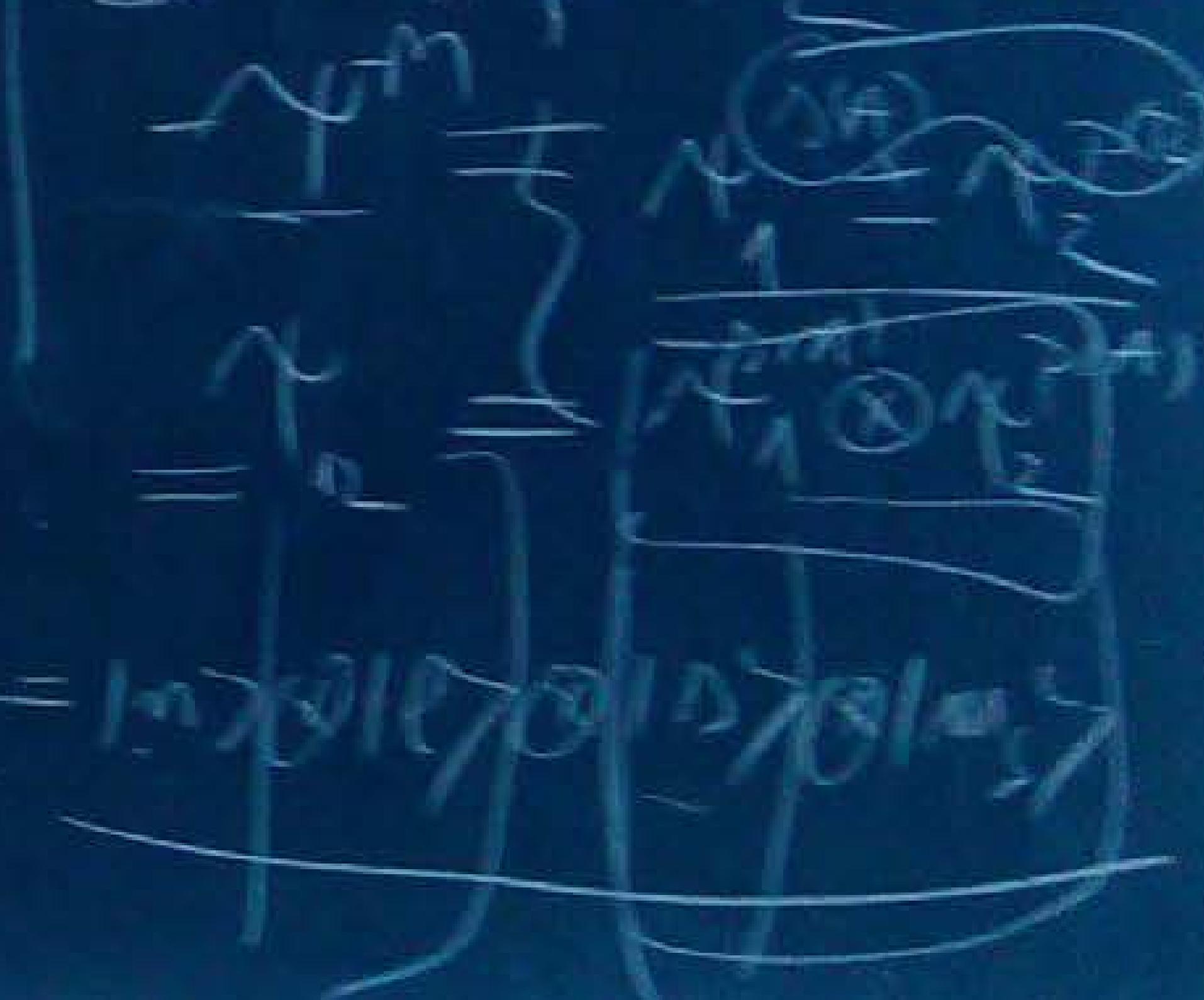
ACCORP
= $\langle \psi_1 | \psi_2 \rangle$
($\psi_1 | \psi_2$)

$\ln \langle \psi_1 | \psi_2 \rangle$

log of $A_{12} = \ln \langle \psi_1 | \psi_2 \rangle$

Spunand
observabil

1



Cosul Molec.

Natura

Quantica a Legăturii Chimice

A, B

Biotanica

$$E_{AB} = \frac{\int \psi_{AB}^* H \psi_{AB} d\tau}{\int \psi_{AB}^* \psi_{AB} d\tau} = \frac{\int (\psi_A c_1 + \psi_B c_2)^* H (\psi_A c_1 + \psi_B c_2) d\tau}{c_1^2 + 2c_1 c_2 S_{AB} + c_2^2}$$

$$\hat{H}_{AB}$$

$$\psi_A$$

$$\psi_B$$

$A \otimes B$

$$\psi_{AB} = c_1 \psi_A + c_2 \psi_B, \quad c_1, c_2 \in \mathbb{R}$$

edulare a intera de!

$$\left\{ \begin{array}{l} \psi = ? \quad (c_1, c_2 = ?) \\ E_{AB} = ? \end{array} \right.$$

$$1 = \int \psi_{AB}^* \psi_{AB} d\tau = \int (c_1 \psi_A + c_2 \psi_B)^* (c_1 \psi_A + c_2 \psi_B) d\tau$$

$$A = \int \psi_A^* \psi_A d\tau = c_1^2 + 2c_1 c_2 S_{AB} + c_2^2$$

$$1 = c_1^2 \int \psi_A^* \psi_A d\tau + 2c_1 c_2 \int \psi_A^* \psi_B d\tau + c_2^2 \int \psi_B^* \psi_B d\tau$$

Cosul Molec.

Natura

Quantica a Legăturii Chimice

interacțiune de schimb

A, B Bistare

$$E_{AB} = \frac{\int \psi_{AB}^* H \psi_{AB} d\tau}{\int \psi_{AB}^* \psi_{AB} d\tau} = \frac{\int (\psi_A c_1 + \psi_B c_2) \hat{H} (\psi_A c_1 + \psi_B c_2) d\tau}{c_1^2 + 2c_1 c_2 S_{AB} + c_2^2}$$

$\hat{H}_{AB}$ ψ_A ψ_B $A \otimes B$

edulare a interactiv?

$$\psi_{AB}^M = c_1 \psi_A + c_2 \psi_B, \quad c_1, c_2 \in \mathbb{R}$$

(int. Coulomb)

$$\int \psi_A \hat{H} \psi_B d\tau = K_{AB}$$

$$\int \psi_B \hat{H} \psi_A d\tau = K_{BA}$$

$$\begin{cases} \psi = ? \quad (c_1, c_2 = ?) \\ E_{AB} = ? \end{cases}$$

$$= \frac{c_1^2 \int \psi_A \hat{H} \psi_A d\tau + c_2^2 \int \psi_B \hat{H} \psi_B d\tau + 2c_1 c_2 \int \psi_A \hat{H} \psi_B d\tau}{c_1^2 + c_2^2 + 2c_1 c_2 S_{AB}}$$

$$A = \int \psi_A^* \psi_A d\tau = c_1^2 + 2c_1 c_2 S_{AB} + c_2^2$$

"A, B" = "A₁, A₂" = "H^{me}₁, H^{me}₂" (H-H, N-N, O-O)

$K_{AB} = K_{BA} = K$ (int. de schimb - Clebsch-Gordan)

$$\psi_{AB} = \frac{c_1^2 S_A + c_2^2 S_B + 2c_1 c_2 K}{c_1^2 + c_2^2 + 2c_1 c_2 S}$$

Coorul Molec. Natura Cuantica a Legaturii Chimice

A, B Born-Haber

$\hat{H}_{AB}$

ψ_A

ψ_B

$A \otimes B$

$$\psi_{AB}^M = c_1 \psi_A + c_2 \psi_B$$

$$\begin{cases} \gamma = ? \\ E_{AB} = ? \end{cases}$$

$$\begin{cases} \gamma = \frac{1}{\sqrt{2}}(\psi_A - \psi_B) \\ c_1, c_2 = ? \\ E_{AB} = S - K \\ E_{AB} = S + K \\ c_1 = c_2 \\ c_1 = -c_2 \end{cases}$$

$$A = \int \psi_A^2 d\tau = c_1^2 + 2c_1 c_2 S + c_2^2$$

$$1 = c_1^2 + c_2^2 \Rightarrow c_1 = \frac{1}{\sqrt{2}}$$

$$\frac{\partial E_{AB}}{\partial c_1} = 0$$

$$\frac{\partial E_{AB}}{\partial c_2} = 0$$

$$\bar{E}_{AB} = \frac{c_1^2 S_A + c_2^2 S_B + 2c_1 c_2 K}{c_1^2 + c_2^2 + 2c_1 c_2 S}$$

$$\begin{vmatrix} S-E & K \\ K & S-E \end{vmatrix} = 0 \quad (S-E)^2 = K^2 \quad S-E = \pm K \quad E = S \pm K$$

$A-A$
 $\psi_A \psi_A$

$$S_A = S_B = S$$

$$c_1(S_A - E) + c_2(K - ES) = 0$$

$$c_1(K - ES) + c_2(S_B - E) = 0$$

$$\begin{cases} c_1(S-E) + c_2 K = 0 \\ c_1 K + c_2(S-E) = 0 \end{cases} \Rightarrow c_1 = -c_2 \frac{K}{S-E}$$

$$c_1^2 S_A + c_2^2 S_B + 2c_1 c_2 K = E(c_1^2 + c_2^2 + 2c_1 c_2 S)$$

Natura Quantica e Legittimo Chimica

IV P. General al Bonding (Pauli)

Ψ^M generalo = Ant. Symmetric
 (Spin) (X) (Spin)

$$\Psi_{AB}^M = c_1 \psi_A + c_2 \psi_B$$

$$\begin{cases} \psi = \frac{1}{\sqrt{2}}(\psi_A - \psi_B) \\ c_1, c_2 = ? \\ E = \dots - K \\ E = \dots + K \\ \psi_{AB} = \frac{1}{\sqrt{2}}(\psi_A + \psi_B) \end{cases}$$

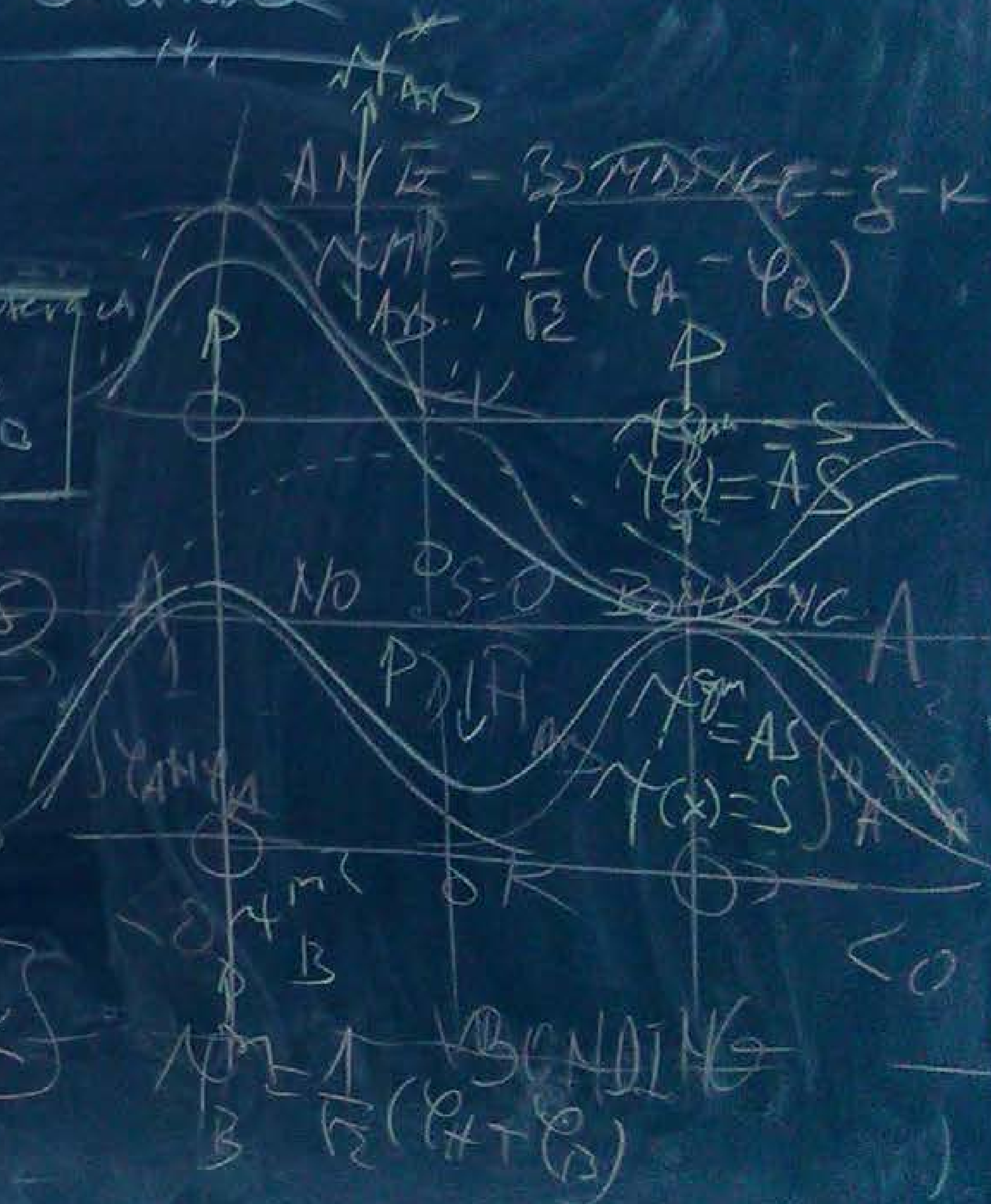
$$J, K < 0$$

$$\frac{\partial E_{AB}}{\partial c_1} = 0$$

$$\frac{\partial E_{AB}}{\partial c_2} = 0$$

$$E = J$$

$$E = J + K$$



Legolova Covalent

- Principle limited (pr. Pauli) | 2 principle (Hund Rules)
- Introduces OM leg in ant by Pauli $\sigma, \sigma^*, \pi, \pi^*$ | 4 layers
 on structure for no bonding & antibonding (pp) (pp) Diatomic Bonding
- Diagrams OM per configuration (sp) | 1 layer
 OA 1s, 2s, 2p
- Apply to molec. (per Pauli diagram OM/1s2s2p) H_2, F_2, N_2, HF | 4 layers (3 same, 1 another)
 NO Diagrams of bonding molecules
 NO Covalent Bonding

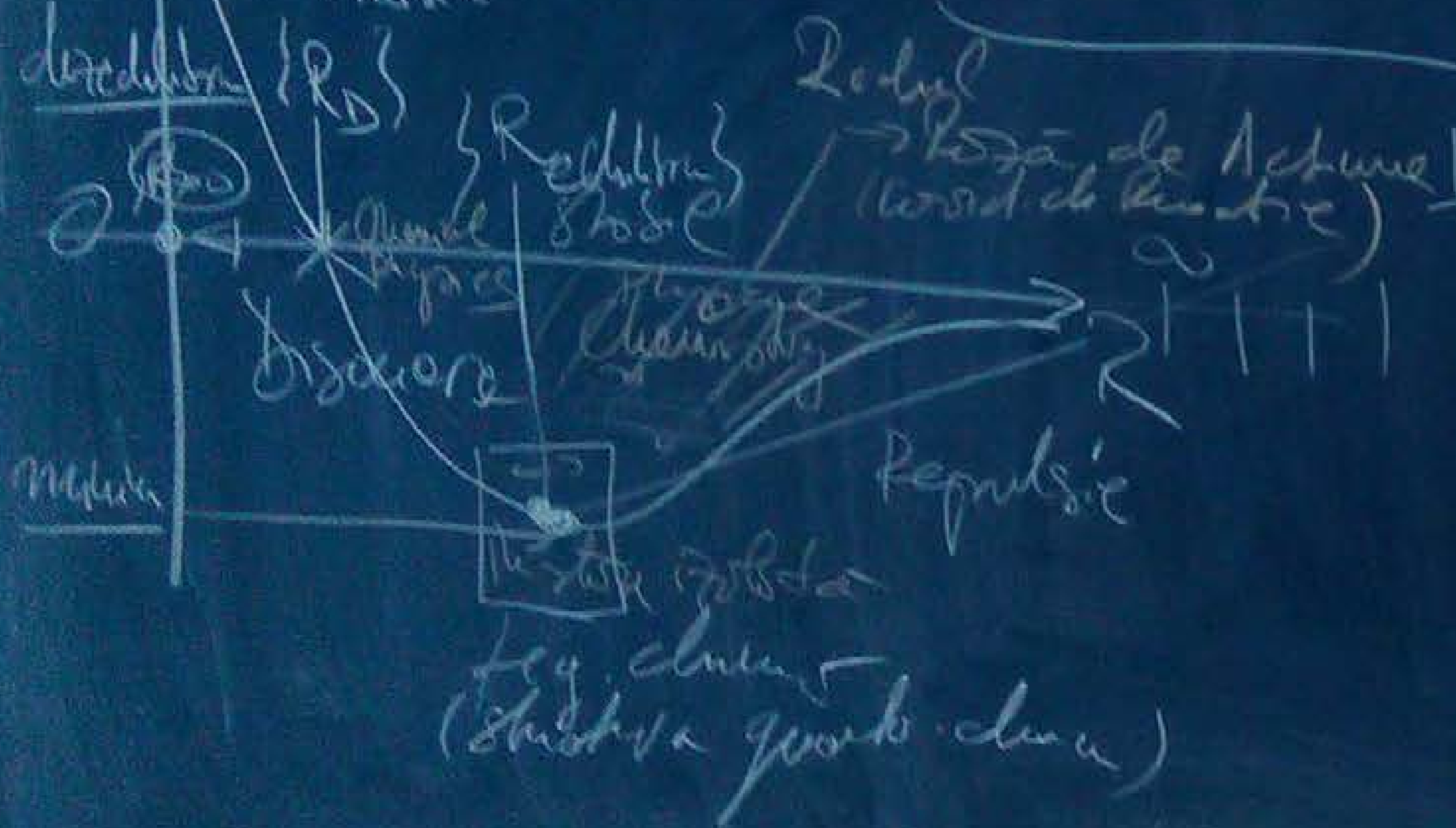
Structura Cuantică a Moleculor (Bintonia)

$V(R)$ pot. de interacție
moleculare
(Sf. potențial
cîm și electron)
electron
nucleu

Hamiltonianul
molecular

electroni și
nucleu

Aproximarea Adiabatică



tipuri de mișcare / energii
intra-moleculare
(structurale)

molec. cu
ordonare
(post-interacție
componente)

$$\Delta p \frac{\Delta x}{a} \sim \frac{h}{a} \Rightarrow \Delta p = \frac{h}{a}$$

Structura Cuantică a Moleculilor (Bintonica)

Tipurile de energii din Moleculă

Comportamentul plechometric (!)

$$\{RS\} \sim a_n \sim \Delta x$$

- Energie electronică / nivel electronic E_e
- Energie de vibrație E_v
- Energie de rotație E_r

$$E_e \sim T_e \sim \frac{(\Delta p)^2}{2m_e} \sim \frac{h^2}{2a^2m_e} \sim eV$$

$$E_v \sim \frac{h\nu}{m_{HCl}} \sim \frac{h}{m_{HCl}} \sqrt{\frac{k_e}{m_{HCl}}} = \frac{h}{m_{HCl}} \left(\frac{E_e}{a^2 m_{HCl}} \right)^{1/2} = \frac{h}{m_{HCl}} \left(\frac{h^2}{2a^2 m_e} \frac{1}{a^2 m_{HCl}} \right)^{1/2} = \frac{h}{m_{HCl}} \left(\frac{h^2}{2a^4 m_e m_{HCl}} \right)^{1/2} = \frac{h}{m_{HCl}} \left(\frac{h^2}{2a^4 m_e m_{HCl}} \right)^{1/2} = \frac{h}{m_{HCl}} \left(\frac{h^2}{2a^4 m_e m_{HCl}} \right)^{1/2}$$

$V(\text{atomic})$ Atomii

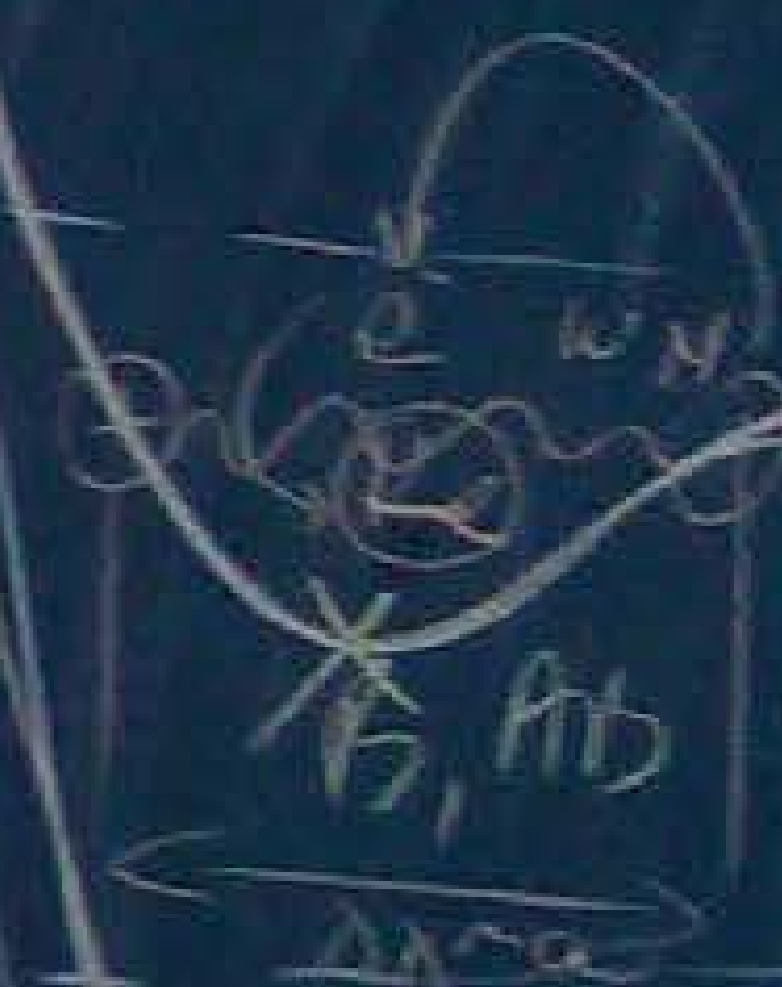
E

moleculă

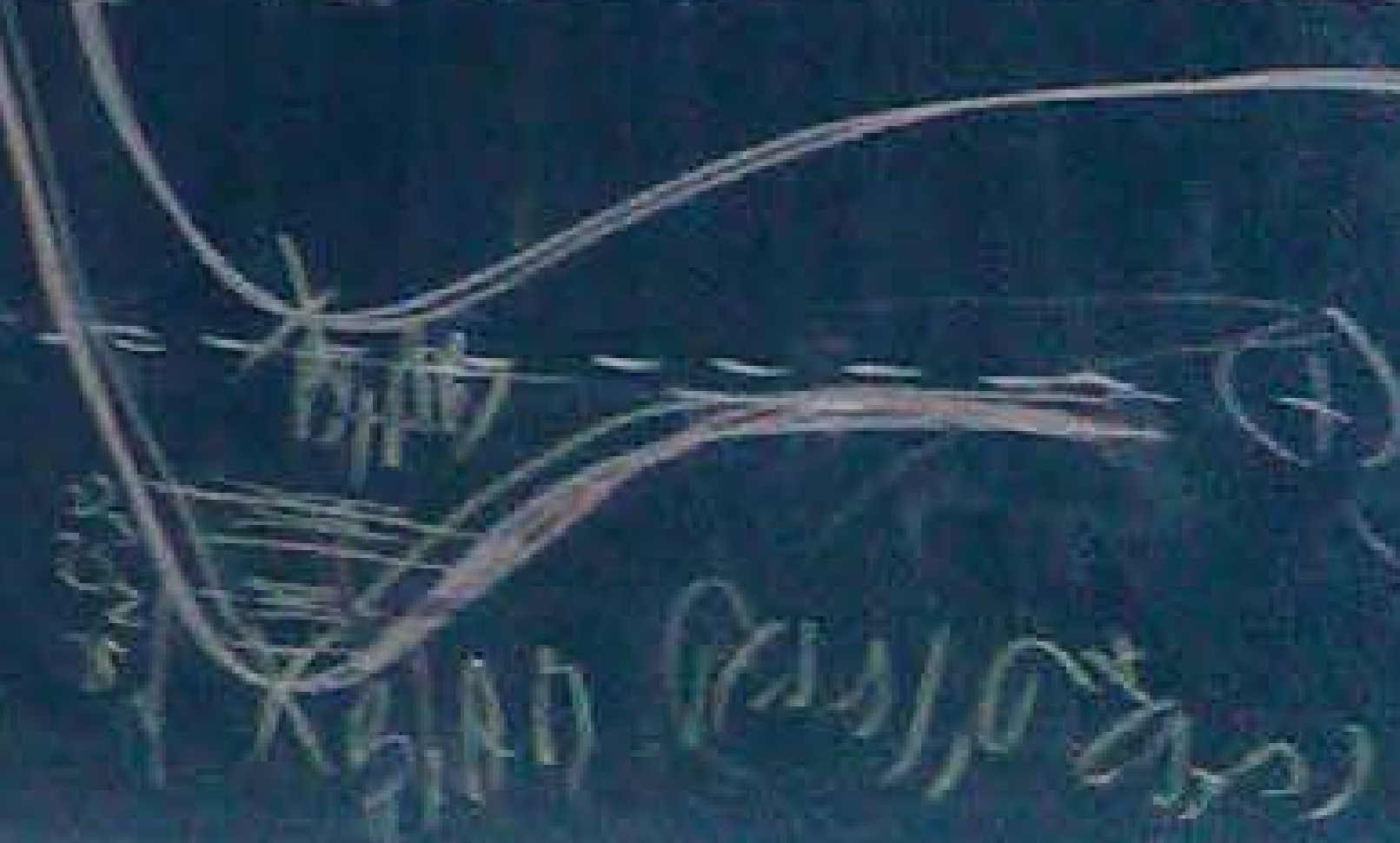
$$E_w(a=0) = \frac{1}{2} h \omega$$

$$\frac{m_e}{m_H} \sim 10^{-3} - 10^{-4}$$

$(n=1)$



$$E_e \sim \frac{k_e (\Delta x)^2}{2m_e a^2}$$



$$\Delta p \Delta x \sim \hbar$$

$$\Delta p \sim \hbar / \Delta x$$

Structura Cuantică a Moleculor (Bontomice)

Tipurile de energii din Moleculă

$$E_r \sim \frac{(\text{mom. orbital})^2}{\text{mom. de inerție}} \sim \frac{(\hbar p)^2}{M_H \cdot a^2} \sim \frac{(\Delta p \Delta x)^2}{M_H a^2}$$

$$\sim \frac{\hbar^2}{M_H a^2} \sim \left(\frac{\hbar^2}{a^2 m_p} \right) \cdot \frac{m_e}{M_H} \sim E_e \cdot \left(\frac{m_p}{M_H} \right) \sim \frac{1}{10000} E_e$$

$E_e \gg E_v \gg E_r$

$$1 : 10^{-2} : 10^{-4}$$

$$T_e \sim T_e \sim \frac{(\Delta p)^2}{2m_e} \sim \frac{\hbar^2}{2a^2 m_e} \sim \text{eV}$$

$$E_v \sim \hbar \omega_{\text{vib}} = \hbar \sqrt{\frac{k_e}{m}} = \hbar \left(\frac{E_e}{a^2 m_H} \right)^{1/2}$$

$$= E_e \sqrt{\frac{1}{10^4}} \sim \frac{1}{100} E_e$$

$$= \hbar \left(\frac{\hbar^2}{2m_p a^2} \cdot \frac{1}{a^2 m_H} \right)^{1/2} = \left(\frac{\hbar^2}{a^4} \right)^{1/2} \left(\frac{1}{2m_p m_H} \right)^{1/2}$$

V(atomic) Atomii

E

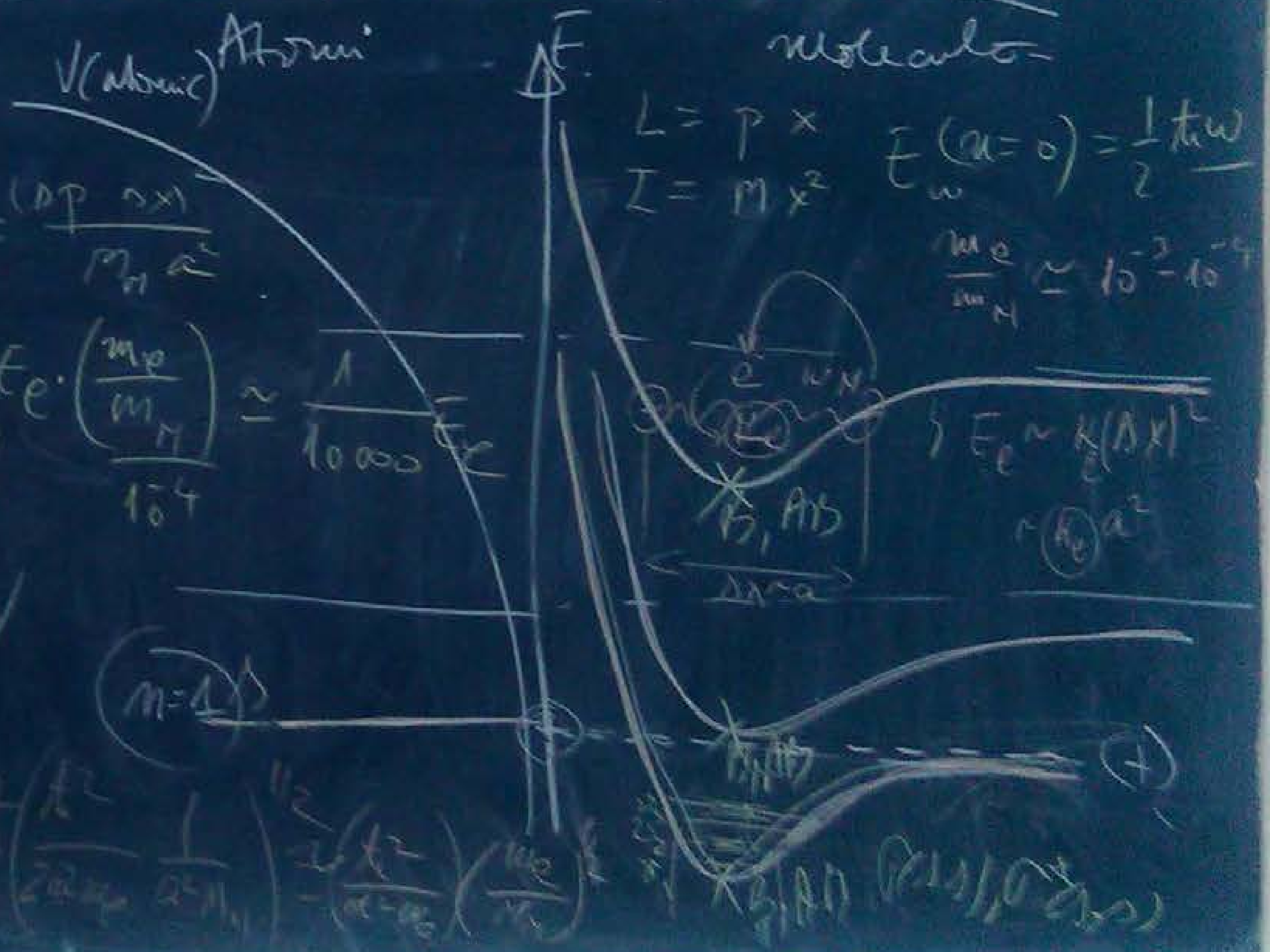
Moleculă

$$L = p \times r$$

$$I = M r^2$$

$$E_w(u=0) = \frac{1}{2} \frac{\hbar^2 \omega}{I}$$

$$\frac{m_e}{m_H} \sim 10^{-3} - 10^{-4}$$



$$E_e \sim \frac{\hbar^2}{a^2 m_e}$$

Electron spin

Studi Spectroscopic

Structura Găsită a Moleculor (Biotonica)

Hamiltonian Molec
in Approx. Adiabatic

Born-Oppenheimer

$$\left\{ \begin{array}{l} \hat{H}_e \psi_e(r, R) = E_e \psi_e(r, R) \\ \hat{H}_n \phi_n(R) = E_n \phi_n(R) \end{array} \right. \Rightarrow \left\{ \begin{array}{l} [\hat{T}_e + \hat{V}_{eN}] \psi_e(r, R) = E_e \psi_e(r, R) \\ [\hat{T}_N + \hat{V}_{eN}] \phi_n(R) = E_n \phi_n(R) \end{array} \right.$$

$\{r\} \rightarrow$ coord. e^-
 $\{R\} \rightarrow$ coord. N^+

$\hat{H}_{molec} \psi(r, R) = E \psi(r, R)$

$\psi(r, R) = \sum_n \phi_n(R) \psi_n(r, R)$

Molec. NT e^- $\{r, R\}$

Energy Molecular

$$\hat{H}_n = -\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + \left[-\frac{\hbar^2}{2M_N} \sum_{\alpha=1}^N \nabla_{\alpha}^2 \right] + V(r, R)$$

Energy de
Baza Găsită
Lărgă, întregul e^-

$V(r, R) = \sum_{i=1}^N \frac{e^2}{r_{ij}}$

1 = (i < j)
Propriet. $(e^- - e^-)$
termolecular
ale molecul

termen
Coulombic
 $\sum_{\alpha \neq \beta} \frac{z_{\alpha} z_{\beta}}{R_{\alpha\beta}} + \sum_{1 \leq \alpha < \beta} \frac{z_{\alpha} z_{\beta}}{R_{\alpha\beta}}$

Studi Spectroscopie

Structura Cuantică a Moleculor (Biotonică)

Hamiltonianul Molec
 & aprox. Adiabatic (Born-Oppenheimer)

$$\begin{aligned} \Psi(r, R), E &\rightarrow \left[\hat{T}_e + \hat{V}_{eN}(R) \right] \psi(r, R) = E_e \psi(r, R) \\ \Phi(R), E_{Mol} &\rightarrow \left[\hat{T}_N + \hat{V}_c(R) \right] \Phi(R) = E_{Mol} \Phi(R) \end{aligned}$$

(Energy Molecular) T_e T_N $(\frac{1}{m_e}) \frac{1}{(m_N)} \frac{1}{(e-N)} \frac{1}{(e-N)}$

$\{r\} \rightarrow$ coord. e^-
 $\{R\} \rightarrow$ coord. N^+

$\hat{H}_{Mol} \Psi(r, R) = E \Psi(r, R)$

$\Psi(r, R) = \sum_n \Phi(R) \psi_n(r, R)$

Molec. $\sum_n$ $\Phi(R)$ $\psi_n(r, R)$

NT e^- $\{1, 2, 3\}$

$$\hat{H}_M = -\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + \left[-\frac{\hbar^2}{2M_N} \sum_{\alpha=1}^N \nabla_{\alpha}^2 \right] + V(r, R)$$

$V(r, R) = \sum_{i=1}^N \frac{e^2}{r_{ij}} - \sum_{\alpha=1}^{N_e} \frac{Z_{\alpha} e}{R_{i\alpha}} + \sum_{1 \leq \alpha < \beta}^{N_N} \frac{Z_{\alpha} Z_{\beta}}{R_{\alpha\beta}}$

Potential (e-e) r_{ij} $\sum_{\alpha=1}^{N_e}$ $\sum_{1 \leq \alpha < \beta}^{N_N}$

Introducere la Grupurile de Simetrie Moleculare

Abordarea Clasică

Operatorul Operator de Simetrie $\hat{R}$: $\hat{R} \hat{H} = \hat{H} \hat{R}$ (op. de simetrie la nivel de operator)

pt. un stat dat $\hat{H} \psi = E \psi$
 ~~este propriu~~
 ~~valorii proprii~~

? Val. proprii ale op. $\hat{R}$?

$\hat{R} \psi = (?) \psi$

$$\hat{R} \hat{H} = \hat{H} \hat{R} \quad (\text{op. de simetrie la nivel de operator})$$

$$\hat{H}(\hat{R} \psi) = \hat{H} \hat{R} \psi = \hat{R} \hat{H} \psi = \hat{R}(E \psi) = E(\hat{R} \psi)$$

$$\int \psi^* (\hat{R} \psi) d\tau = E \int \psi^* (\hat{R} \psi) d\tau = E \int (\hat{R} \psi)^* \psi d\tau = E \int (\hat{R} \psi)^* (\hat{R} \psi) d\tau$$

$$= \int (\psi^* \psi) d\tau = 1 \Rightarrow \hat{R} \psi = (\pm) \psi$$

$$\Rightarrow \begin{pmatrix} (?) \\ \text{op. simetria} \end{pmatrix} = \begin{pmatrix} + \\ - \end{pmatrix} 1$$

(Caractere de simetrie)

= op. de simetrie este caracteristic

Ord. de simetrie

$$= \int (\psi^* \psi) d\tau$$

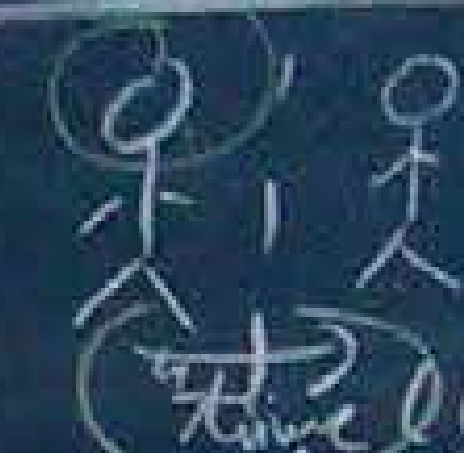
$$\hat{R} \psi = (\pm) \psi$$

vector (fct) propriu!!!
caracter de val. proprii

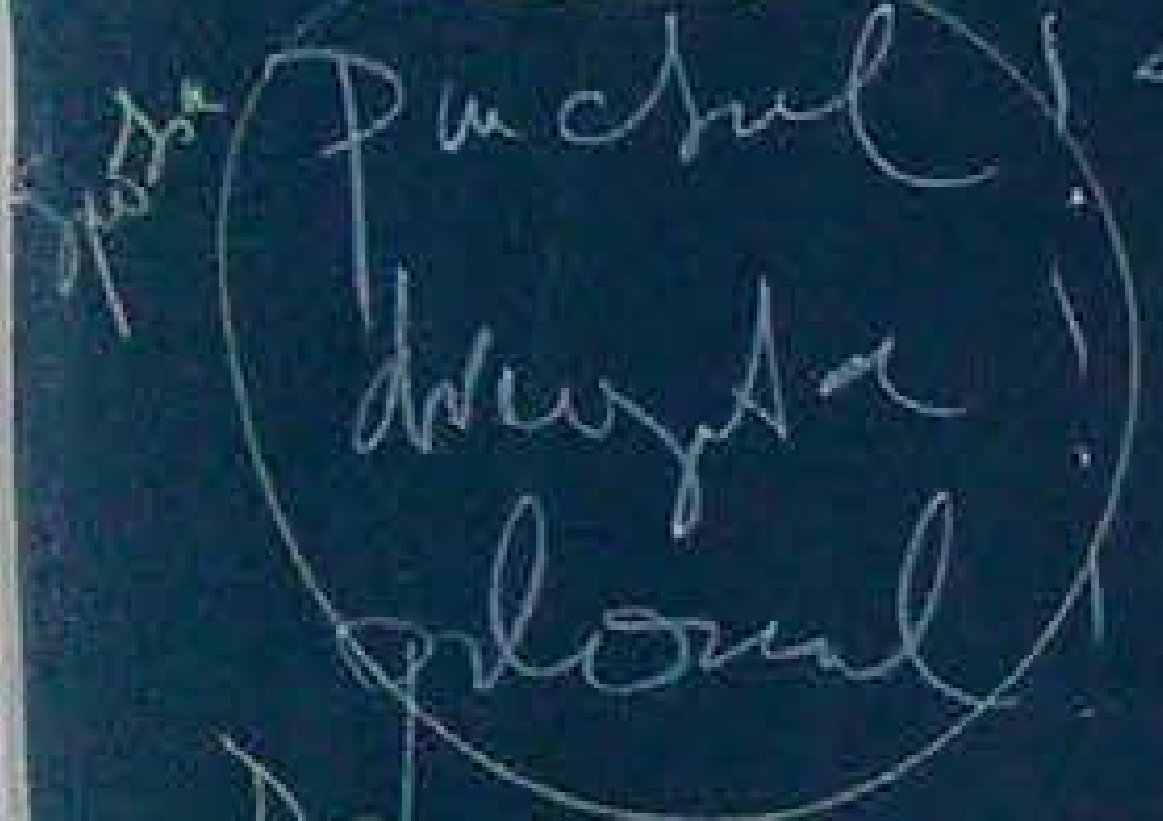
Introducere la Grupurile de Simetrie Moleculare

* Elemente de Simetrie

Vs. Operatii de Simetrie



Amplas



Se desprinde

foto de el de simetrie

identitate ($\hat{E}$)
Inversie ($\hat{i}$)

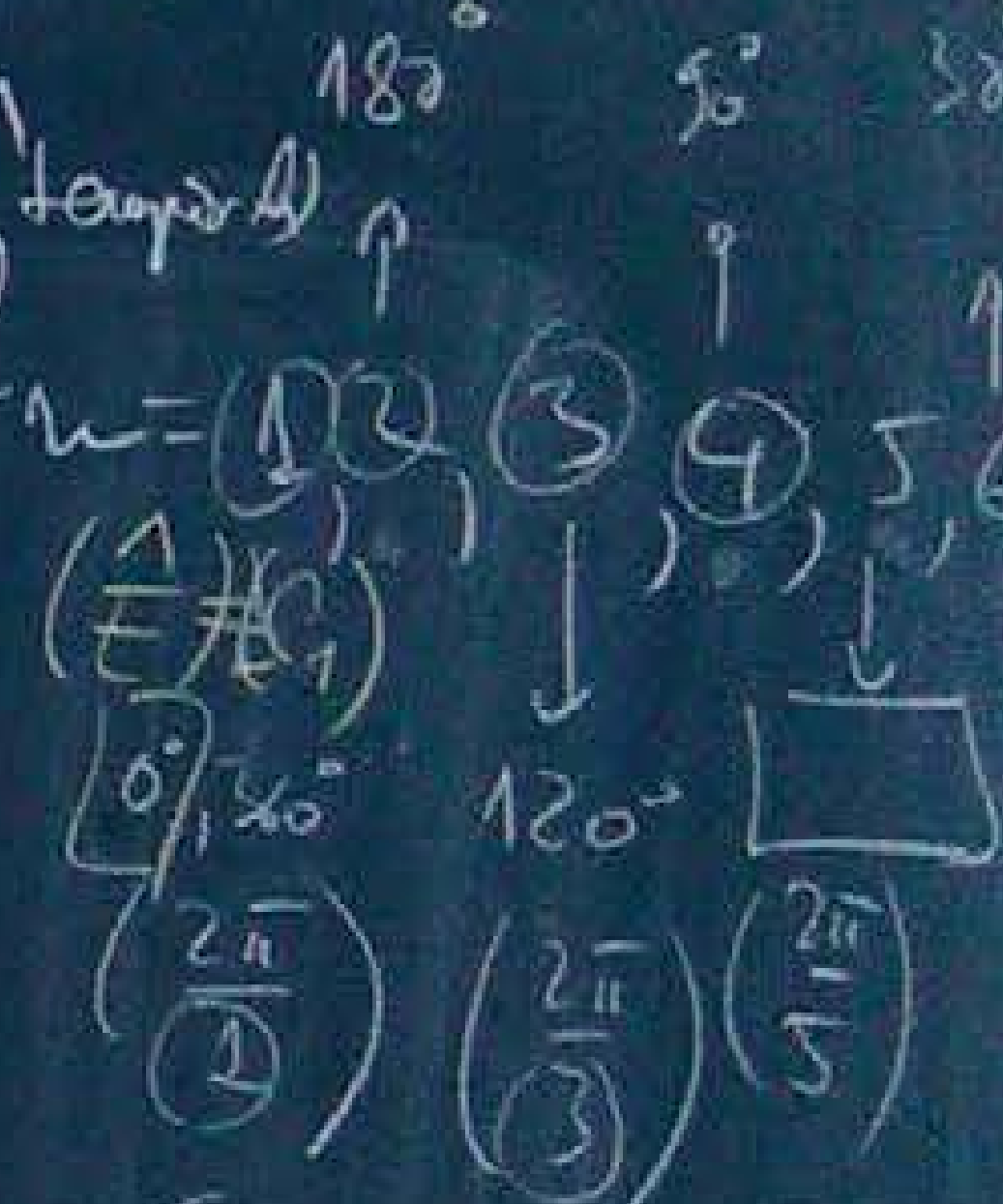
Rotatii

Reflexii ($\hat{\sigma}$)

proprie (doua Rotatii)

improprie (Rotatie + Inversie)

$$\hat{S}_{n=2k} = \hat{C}_{n=2k} \otimes \hat{i}$$

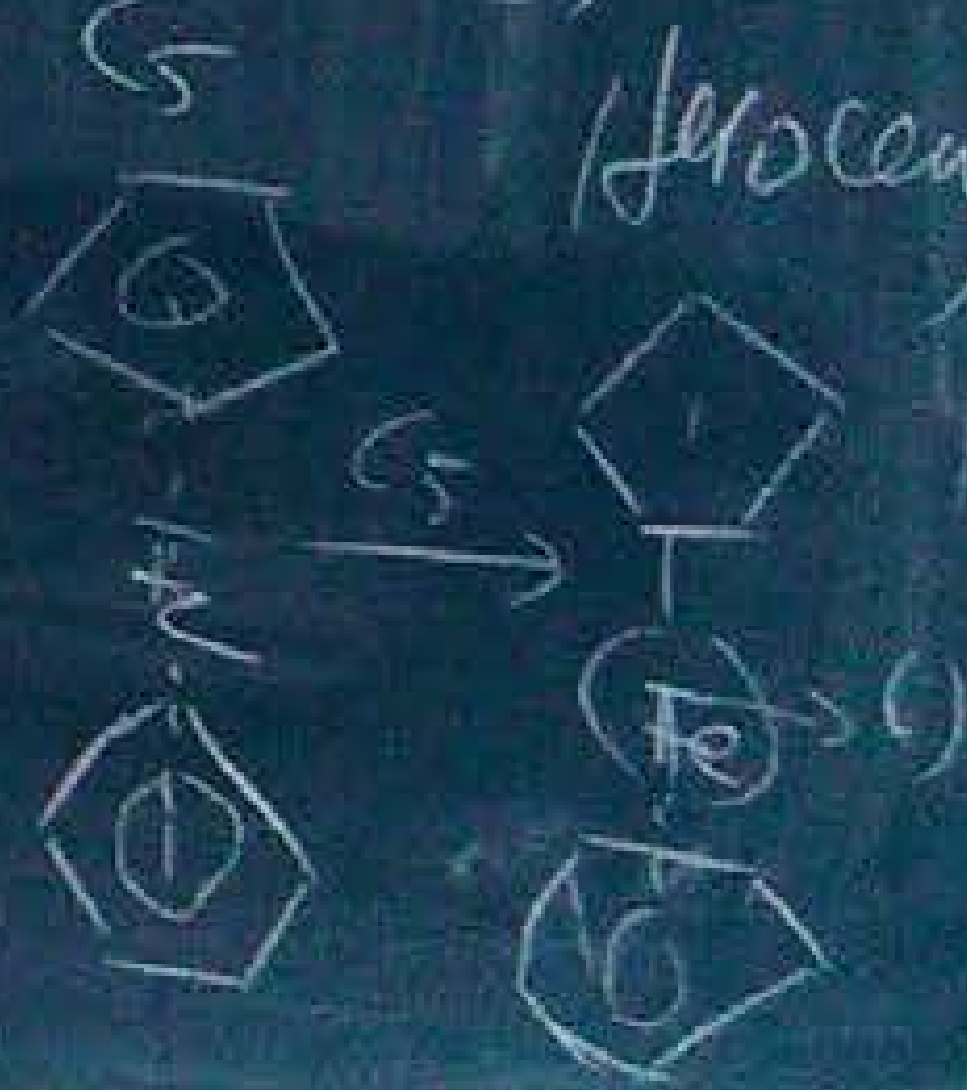
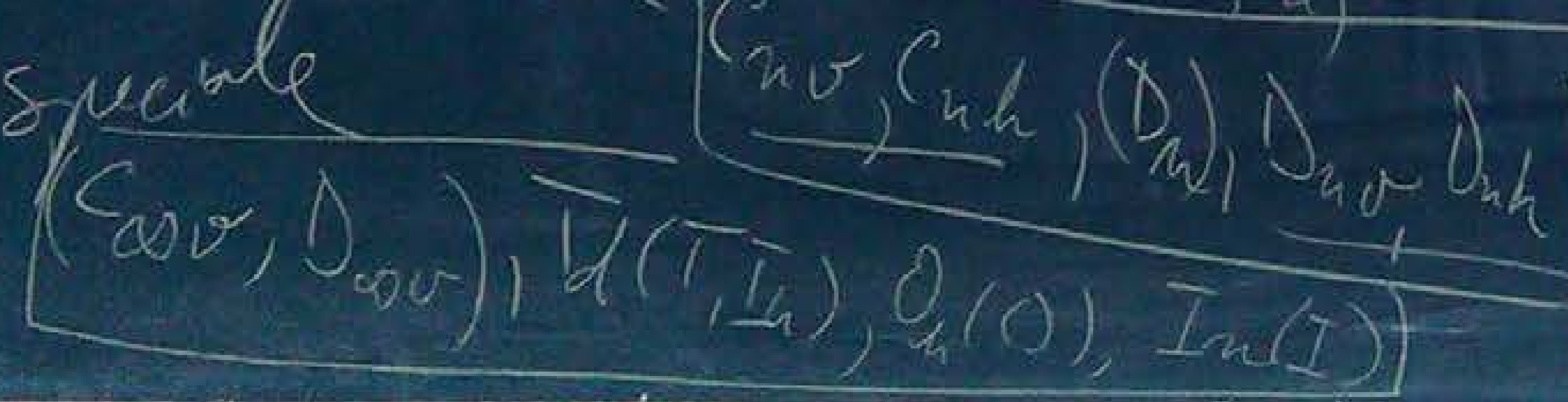
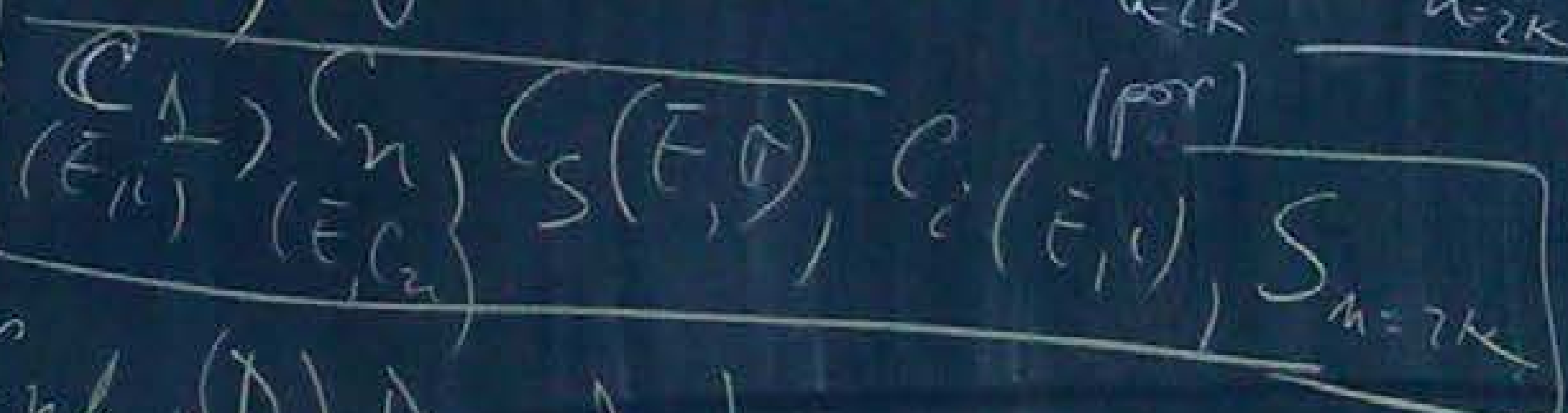


Descrierea grupurilor de simetrie (Scurtar)

I) Cu un singur element de simetrie

II) Cu mai multe elem. de simetrie

III) Grupuri speciale



Introducere la Grupurile de Simetrie Moleculare

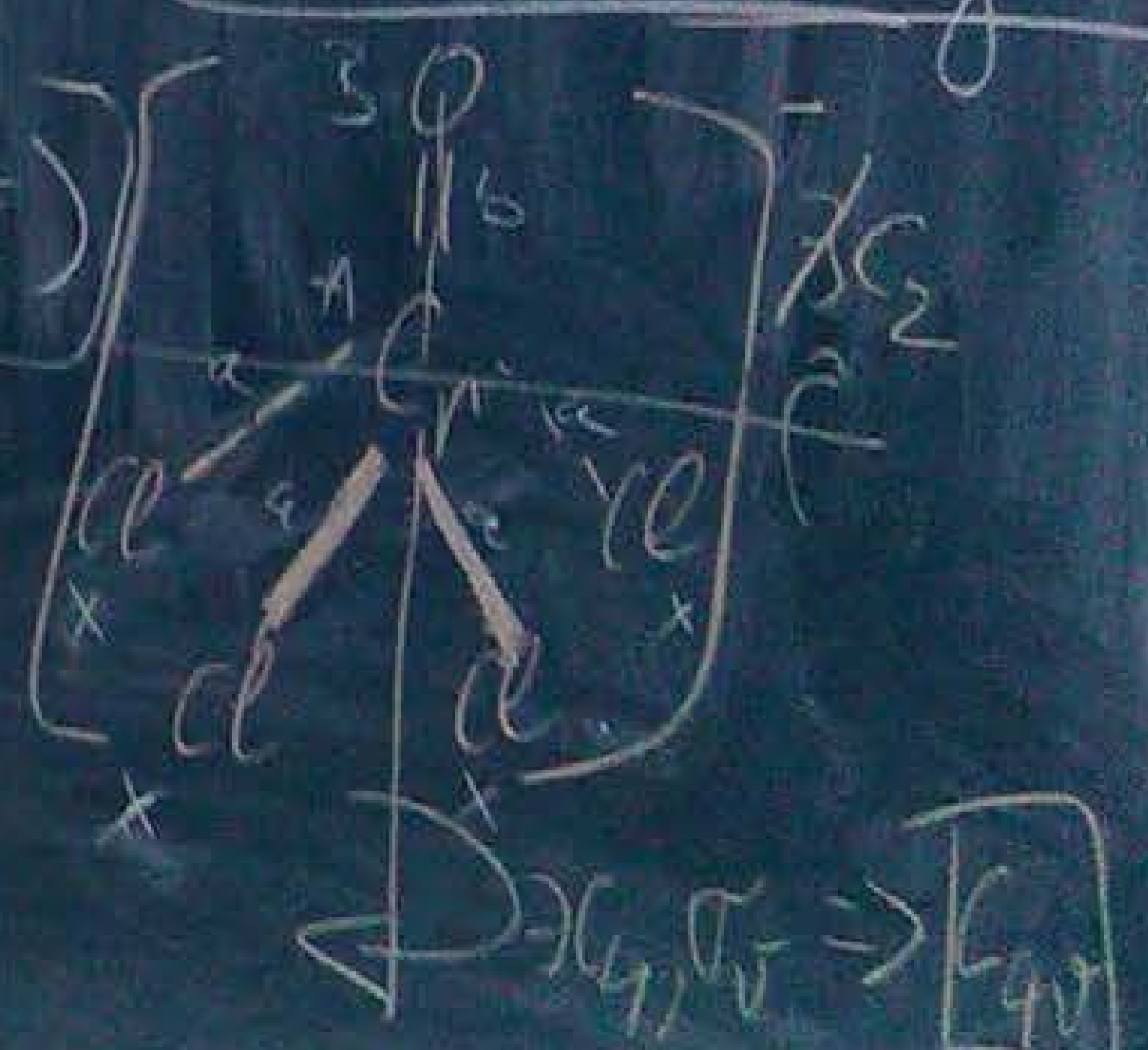
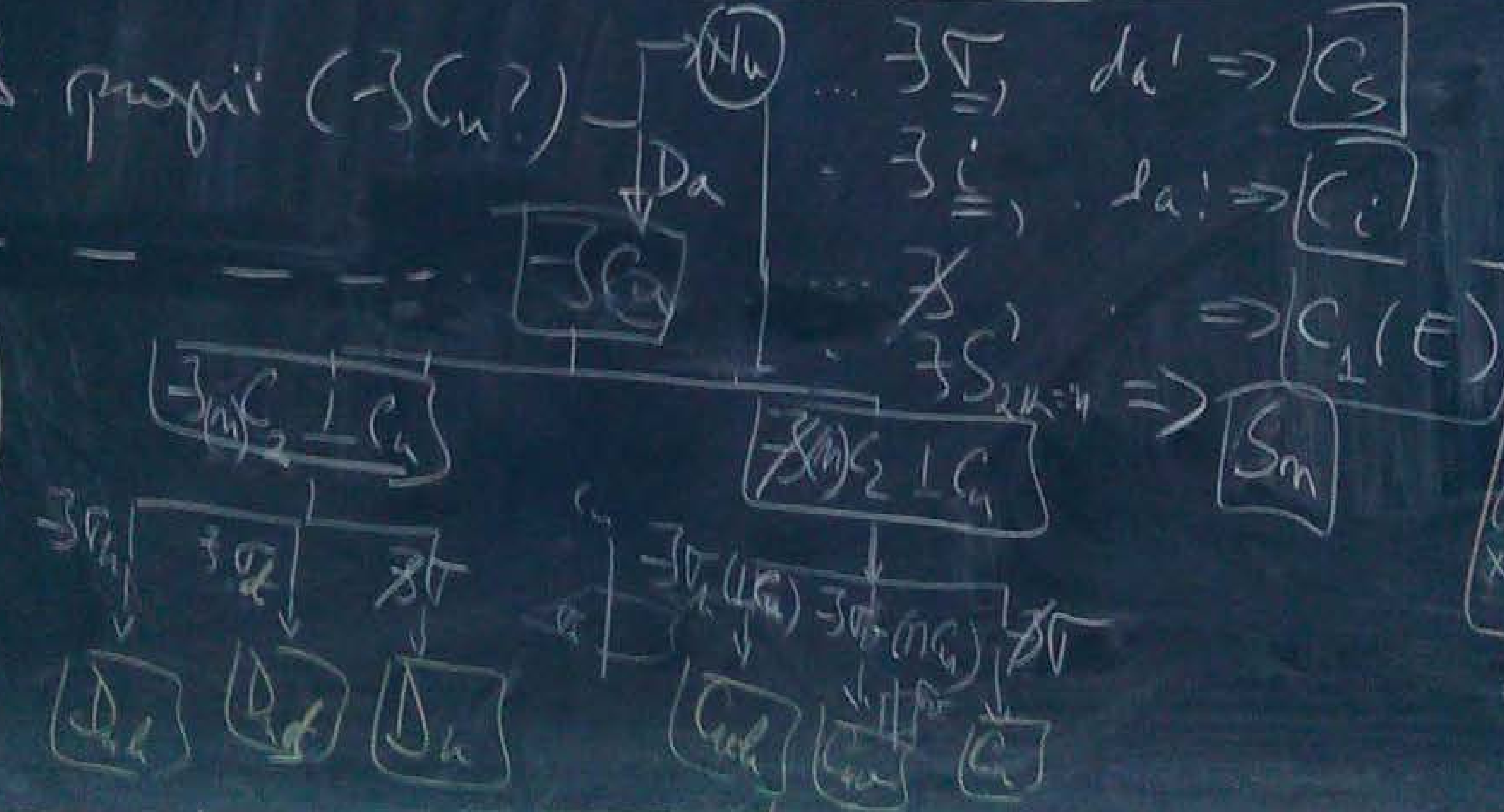
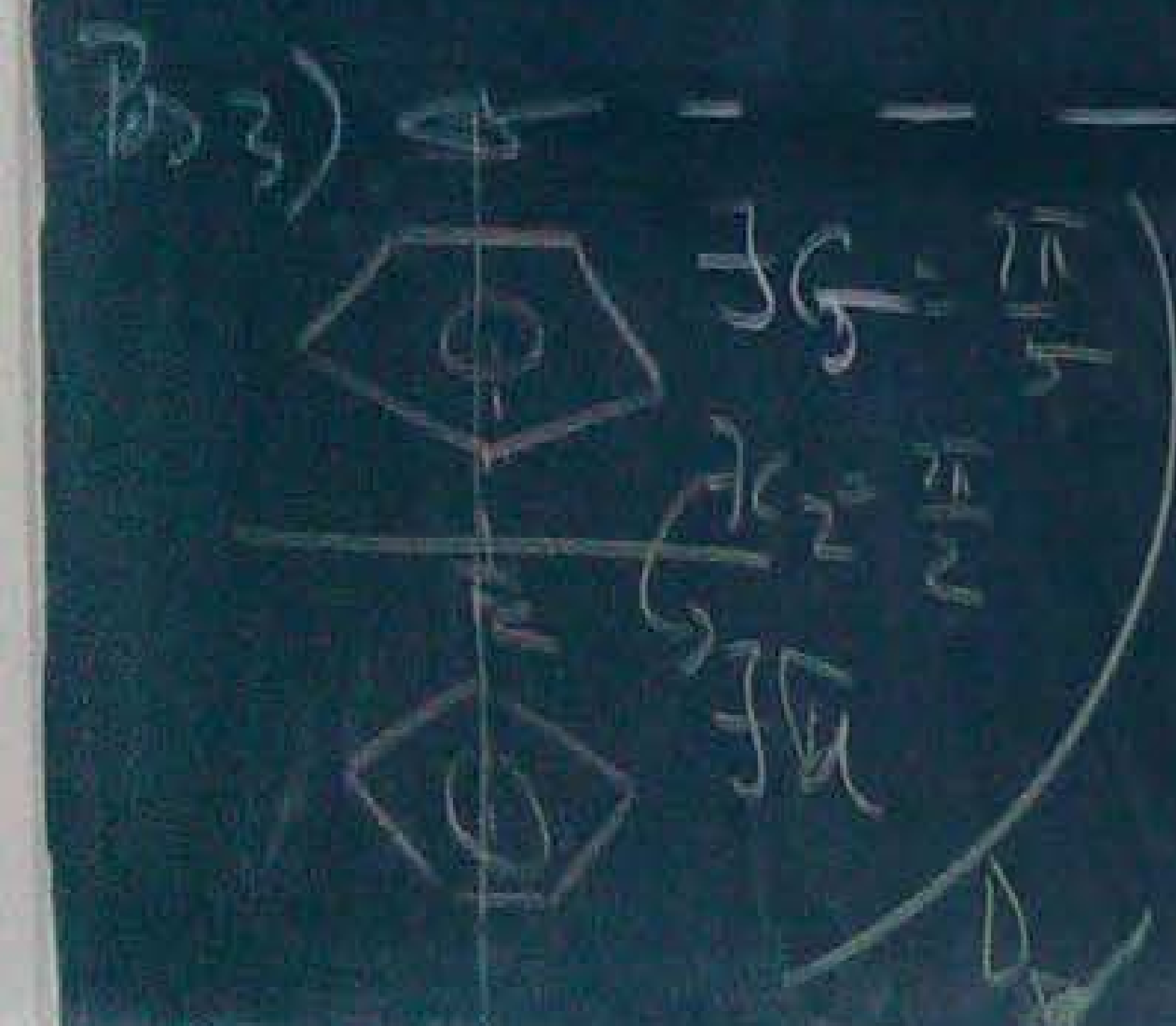
Activitatea este simetrică (pt. molecule / molecular)

Pos 1) Struct. Molec. are ea și gra. un grup special (T, O, I)?

Pe plan matematic / geometric a unei molecule
un punct - atomic
si distanta de legatura

Deci Da → Teoria Grupurilor
Cristalin și de Legătură
(Chem. Analiză și
Chim. Moleculă Organice)

Pos 2) 3 axe de Rot. proprii (3C_n)



Introducere la Grupurile de Simetrie Moleculare

Matricele Op de Simetrie

($\hat{E}$, $\hat{i}$, $\hat{\sigma}$, $\hat{C}_n$) $\rightarrow$ op de simetrie 3D

$\hat{E} \rightarrow$ operatori $\rightarrow$ matrice

$$E_{3D}^{3 \times 3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

matr. dimensională
invariantă

simetrie $\rightarrow$ invariantă

$\sigma_{xz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ -y \\ z \end{pmatrix}$

$\sigma_{xy} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ -z \end{pmatrix}$

$\sigma_{yz} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -x \\ y \\ z \end{pmatrix}$

σ_{xz} σ_{xy} σ_{yz}

$A B = (B^{-1}) A$

(x, y, z)

σ_{xz}

σ_{xy}

σ_{yz}

$$i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

operatori $\rightarrow$ axișe
rot. pat. din
din spațiul
molecular

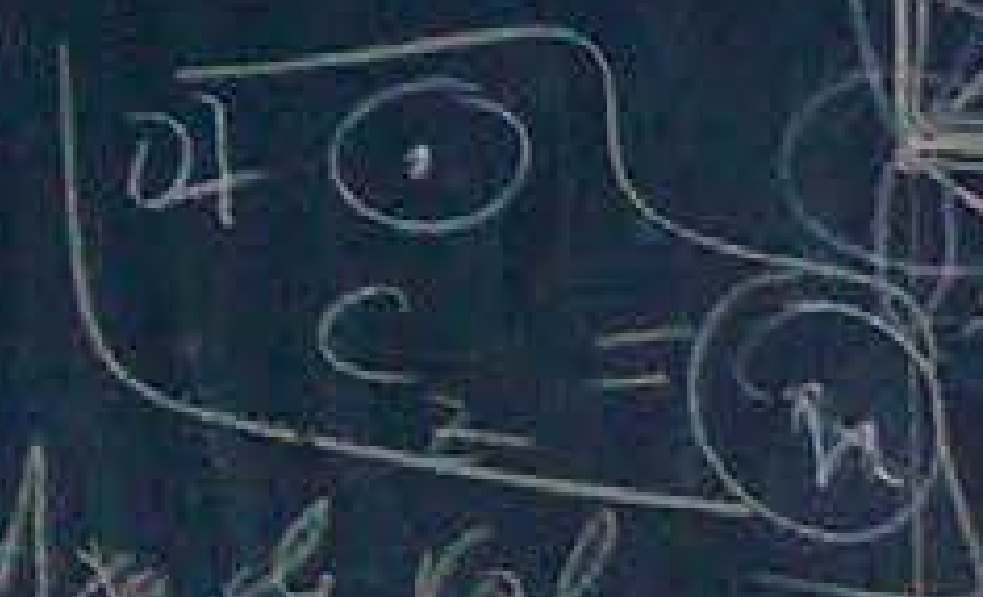
Introducere la Grupurile de Simetrie Moleculare

Matricele Op de Simetrie

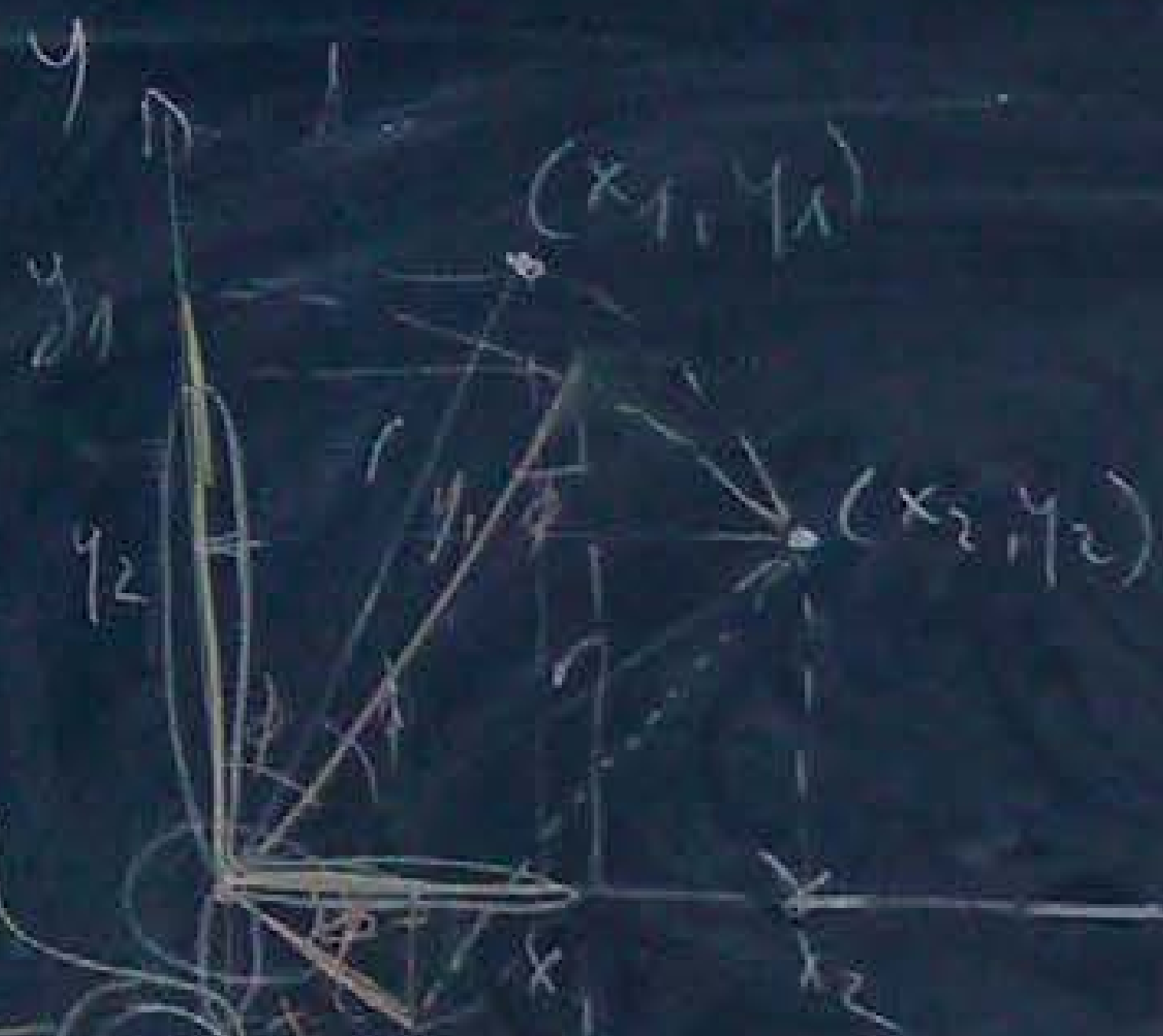
($\hat{E}$, $\hat{i}$, $\hat{\sigma}$, $\hat{C}_n$, $\hat{S}_n$)

$\hat{C}_n$

$$\phi = \frac{2\pi}{n}$$



Axa de rot propriu
x 1 0 z



$$\begin{cases} x_2 = x_1 \cos \phi + y_1 \sin \phi \\ y_2 = -x_1 \sin \phi + y_1 \cos \phi \end{cases}$$

$$S_n = C_n \otimes \sigma_h$$

$$= \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\hat{C}_n = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} = \begin{pmatrix} x_2 \\ y_2 \\ z_1 \end{pmatrix}$$

Matricea Reductibilă
a matricilor Reductibile
asociate op. de simetrie
moleculare existente

Introducere la Grupurile de Simetrie Moleculare

Matricea de Caracter

val proprii ale lui $\hat{\rho}$

$$\phi = \frac{2\pi}{2} = \pi : C_2 = \begin{pmatrix} \cos \pi & \sin \pi & 0 \\ -\sin \pi & \cos \pi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

ex de ligand CH_3 - metan

(2) el (4) $3 \times 3 \rightarrow 2 \times 2$

Matrice Reductibilă

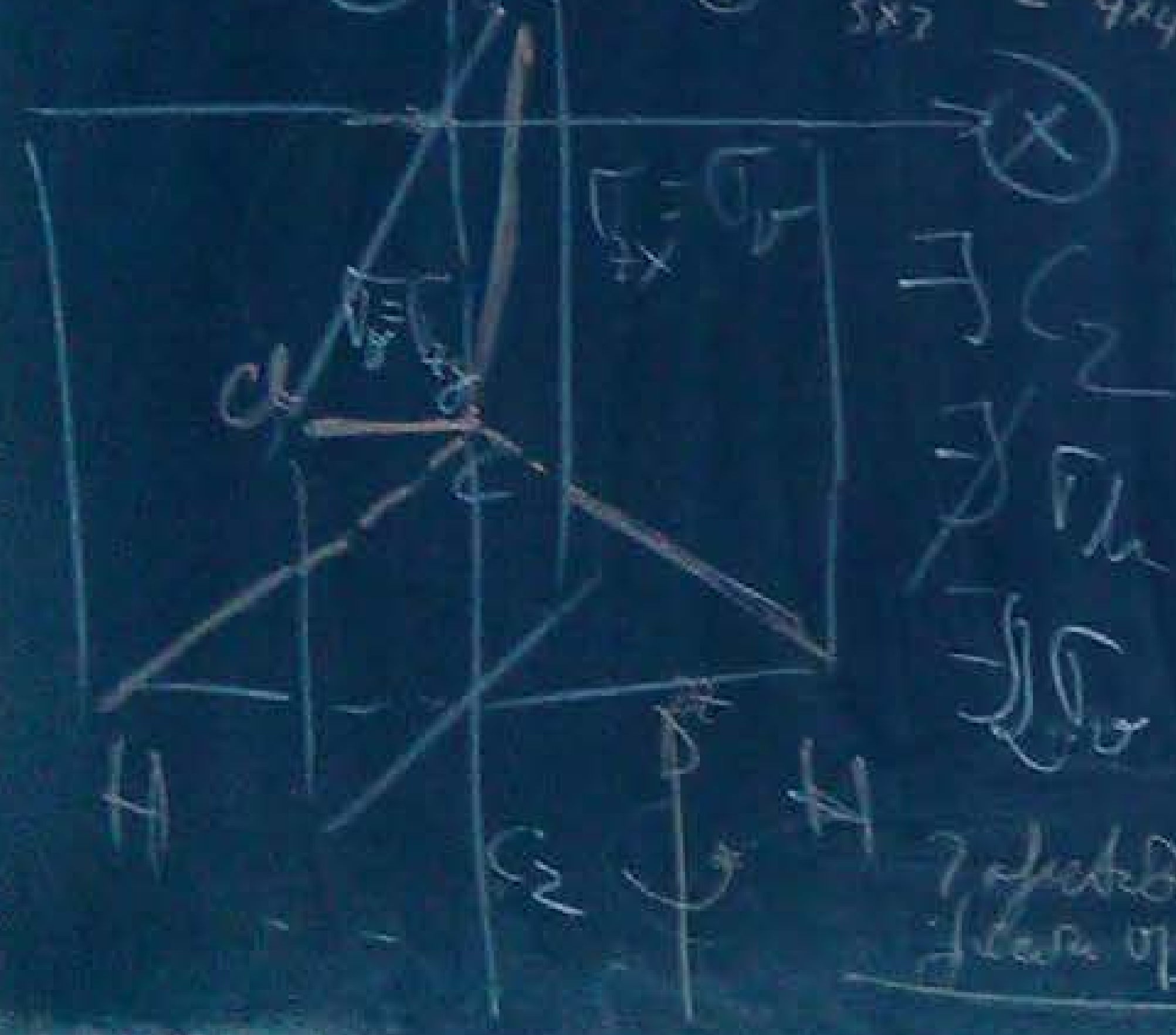
op de simetrie

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



$\hat{C}_2$
 $\hat{\sigma}_v$
 $\hat{\sigma}_v$

C_{2v}

ligand
loos molecule
(de caracter)

Matrice Reductibilă
de caracter

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \end{pmatrix}$$

reducibilă sunt op de simetrie

Descrierea Grupurilor de Simetrie Moleculare (Sumar)

Definitii, Caracteristici
↓ ↓
elemente de simetrie op. de simetrie

in exemple, toti (cu (baza) elem
si op. de simetrie)

Grupuri de simetrie:

E, i, C_n, σ, S_n
 $n=1, 2, 3, 4, 6$
 τ, O, I (V. speciale)
 $C_{nv}, C_{nh}, D_n, D_{nh}, D_{nd}$

↑
identificarea
elem & op.
sim.

Structura și Proprietățile Moleculilor cu Tăla de Caracter

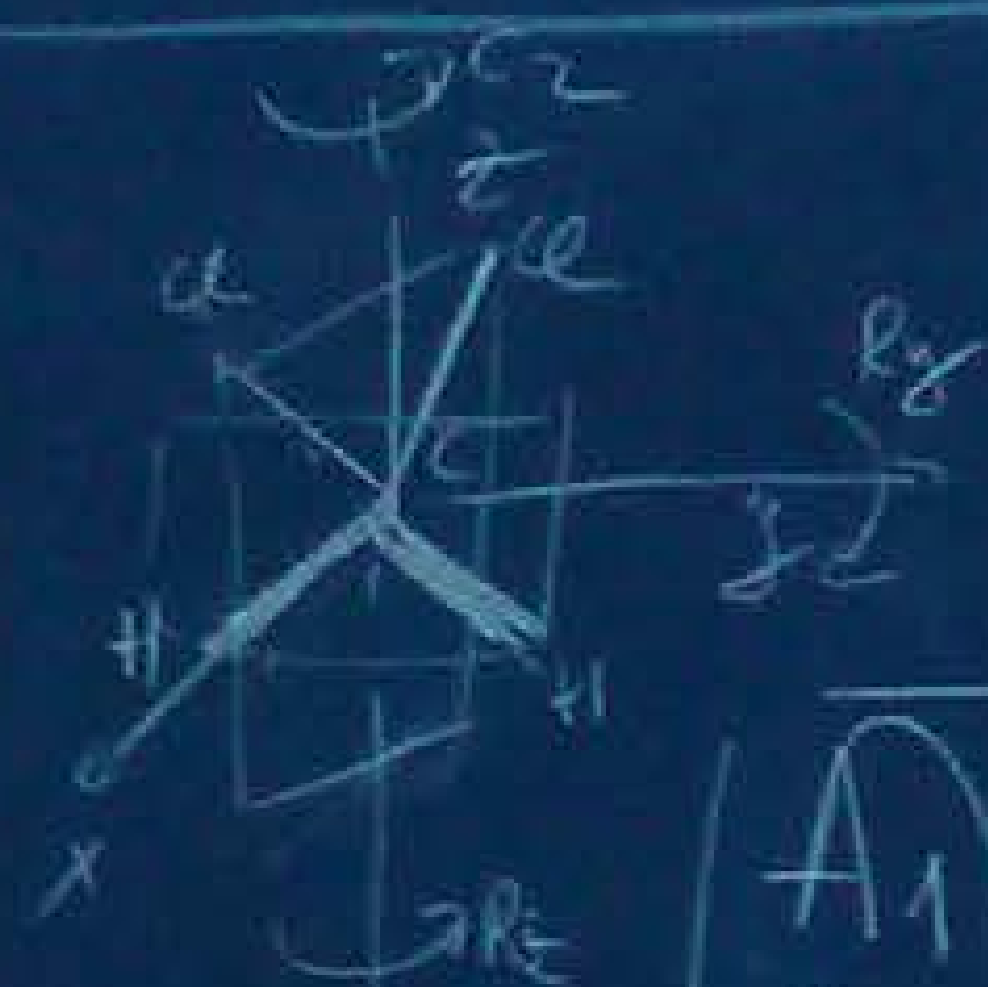
$$(C_{2v}) = \left\{ \begin{matrix} E \\ C_2 \\ \sigma_{xz} \\ \sigma_{yz} \end{matrix} \right\}$$

Matrice
Reducție

matrice de
caractere

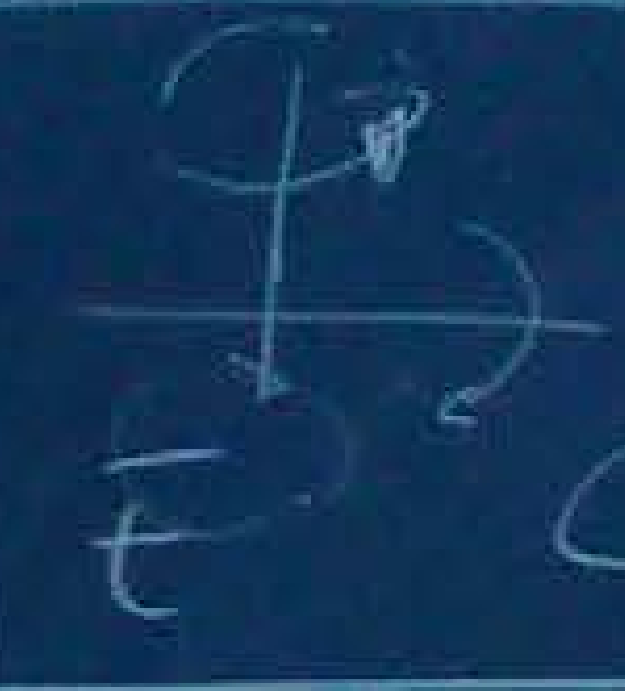
$\begin{pmatrix} R_x \\ R_y \\ R_z \end{pmatrix}$

$$\begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \end{pmatrix} \begin{matrix} B \\ A \end{matrix}$$



Tăla de
Caractere

$\begin{pmatrix} A_1 \\ A_2 \\ B_1 \\ B_2 \end{pmatrix}$



	E	C ₂	σ _{xz}	σ _{yz}
A ₁	1	1	1	1
A ₂	1	1	-1	-1
B ₁	1	-1	1	-1
B ₂	1	-1	-1	1

$\begin{matrix} \mu \\ \text{Repr} \\ \text{de Rădăci} \end{matrix}$ $\begin{matrix} \mu \\ \text{Repr} \\ \text{Binare} \end{matrix}$

$\begin{matrix} x^2, y^2, z^2 \\ R_z \\ x, R_y \\ y, R_x \end{matrix}$ $\begin{matrix} x^2 \\ xy \\ xz \\ yz \end{matrix}$

Reguli
Mulliken

$$\begin{matrix} 1D & A_1, A_2 & \chi(C_2) = +1 \\ 1D & B_1, B_2 & \chi(C_2) = -1 \\ 2D & E & \\ 3D & T_2 & \end{matrix}$$

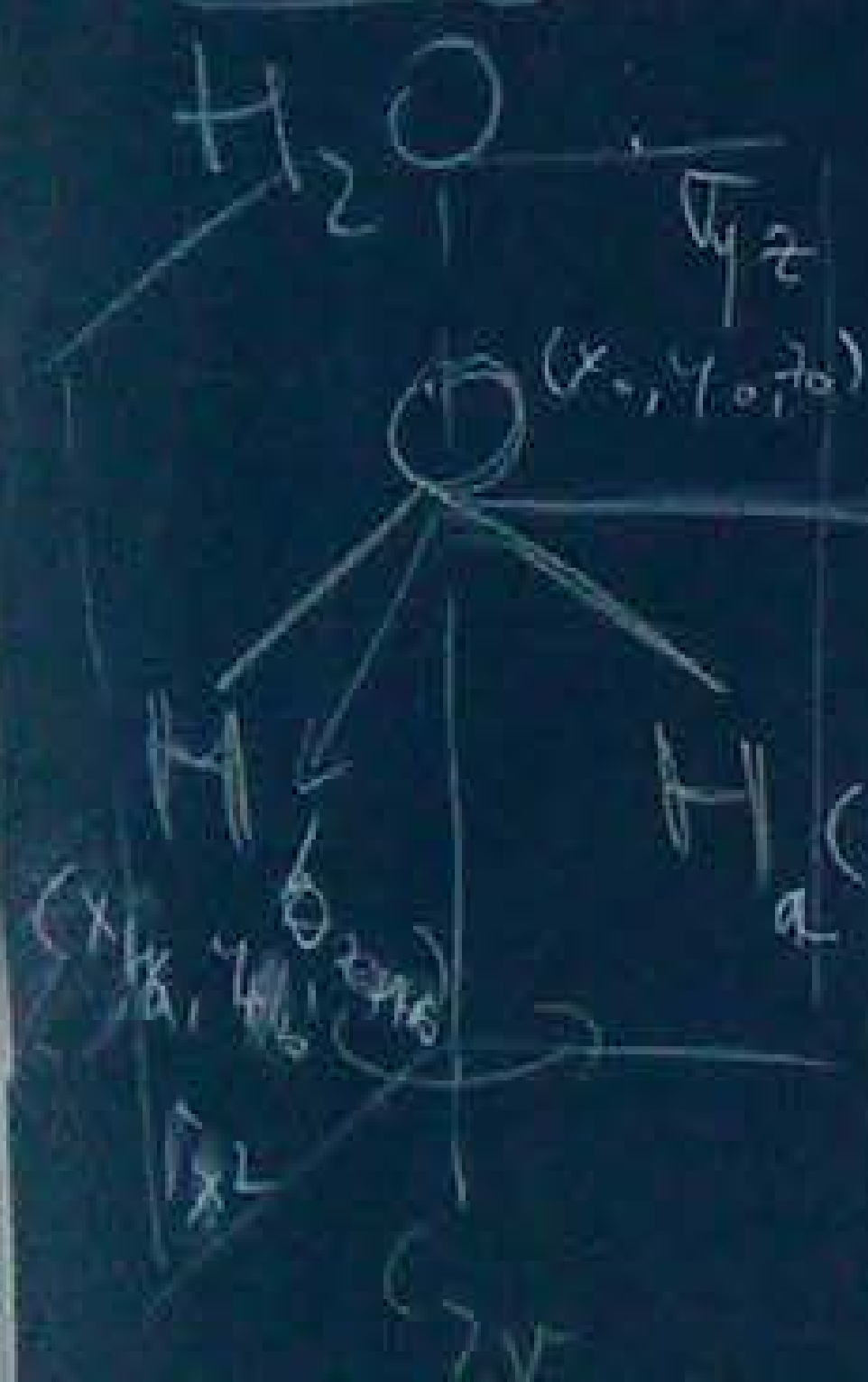
Tăla de
Caractere

+ "matrice de caracter"

matrice de
caractere

Structura și Proprietăți moleculare cu Tabela de Caracterare

? Modulul de vibrație ale unei molecule (Proprietăți)
 1. OIM pt. SA Poliatomic (Structură)



- (I) Se alege o set de Reprezentare
 → coordonate cartezian (x, y, z)
 → funcții de simetrie și funcții de rotație
 → orbitali.

- (II) Se găsește Reprezentare
 totale Γ_{tot} în
 Tabela Reprezentare
 (x, y, z)

- (III) Se deter. $\Gamma = \Gamma_{\text{tot}} - \Gamma_{\text{trans}} - \Gamma_{\text{rot}}$
 (IV) Se extrag
 modurile de vibrație
 1/pe configurație (structură) vibrațională/orbitale 1/QIM

C_{2v}

A ₁	1	1	1	1
A ₂	1	1	-1	-1
B ₁	1	-1	1	-1
B ₂	1	-1	-1	1

E	C ₂	σ _{xz}	σ _{yz}
1	1	1	1
1	1	-1	-1
1	-1	1	-1
1	-1	-1	1

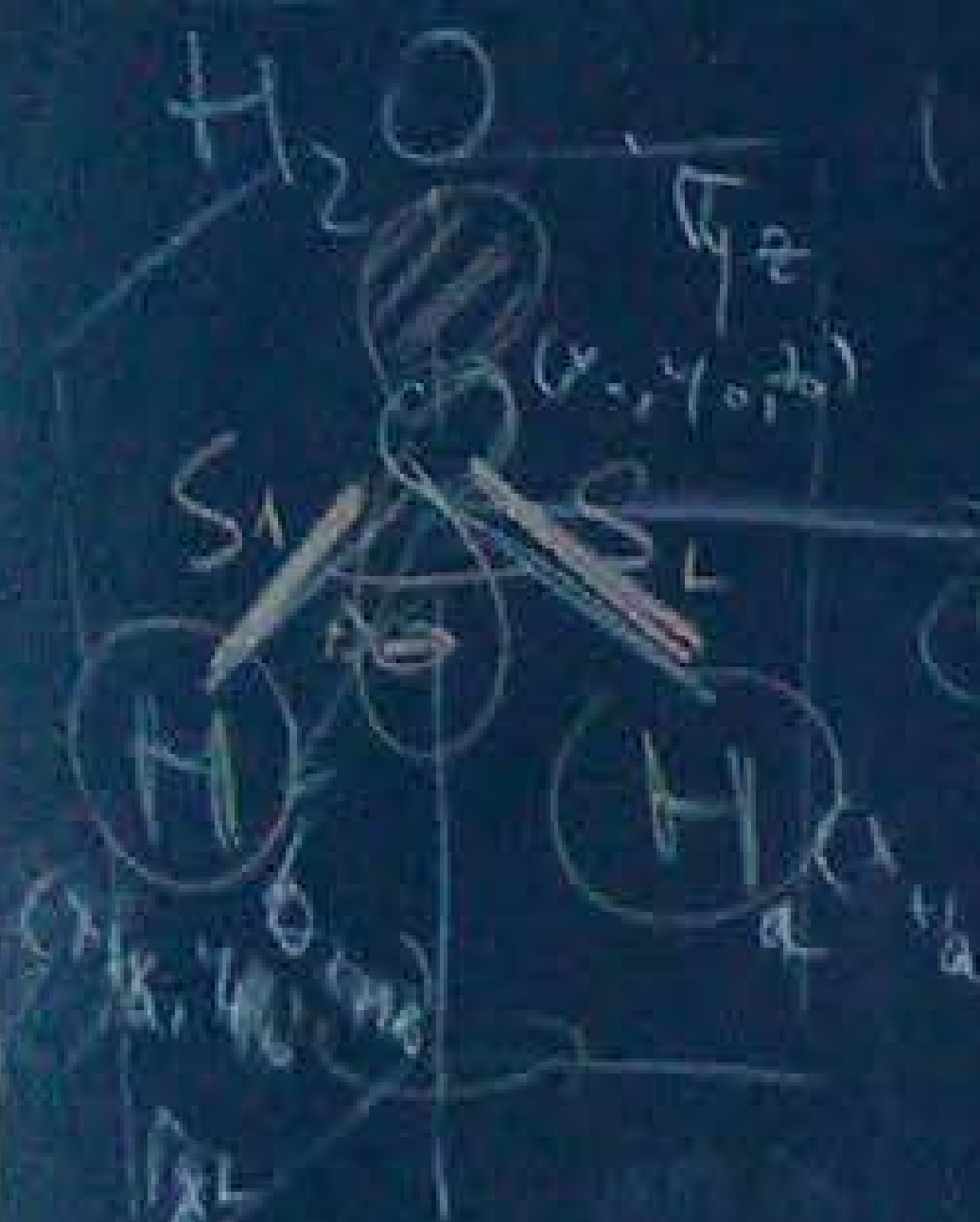
Reprez "Baza" în de Rotatie	Repre Baze "Baza"
z	x ² , y ² , z ²
R _z	xy
x, R _y	xz
y, R _x	yz

+ "moduri de vibrație ale moleculei"

modurile de vibrație ale moleculei

Structura și Proprietățile moleculelor cu Teoria de Caracteri

1) $\Gamma_{H_2O}(\text{total}) = ?$



	E	C_2	σ_{xz}	σ_{yz}
Γ_{xyz}	3	-1	1	1
Atomii necorecte	3	1	1	3
Γ_{H_2O}	9	-1	1	3

C_{2v}
 A_1
 A_2
 B_1
 B_2

	E	C_2	σ_{xz}	σ_{yz}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

μ
 Repre. z
 "Dipole" x
 de Rotatie
 Binare
 Binaire
 x^2, y^2, z^2
 xy
 xz
 yz
 xy, Rx
 yz, Ry
 xy, Rx
 yz, Ry

$\Gamma_{H_2O} = \Gamma_{H_2O} \times \Gamma_{H_2O}$
 $\Gamma_{H_2O} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & -1 \end{pmatrix}$
 $\chi(E) = 3$
 $\chi(C_2) = -1$

Traducere
 Rotatie

modul de
 v. R. R. R.

Structura și Proprietățile moleculelor cu Tăla de Caracter

II

$$\Gamma_{\text{tot}} = \Gamma_{\text{tot}}(\Gamma_{\text{Gr}})$$

$$= \alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 B_1 + \alpha_4 B_2$$

$$= \sum \alpha_i G_i$$

$$\Gamma_{\text{tot}} = \begin{pmatrix} 1 & 1 & 3 \end{pmatrix}$$

$$a_i = \frac{1}{h} \sum g \chi(R) \chi(R)$$

Γ
C_{2v}
A₁
A₂
B₁
B₂

E
1
1
1
1

C₂
1
1
-1
-1

σ_{xz}
1
-1
1
-1

σ_{yz}
1
-1
-1
1

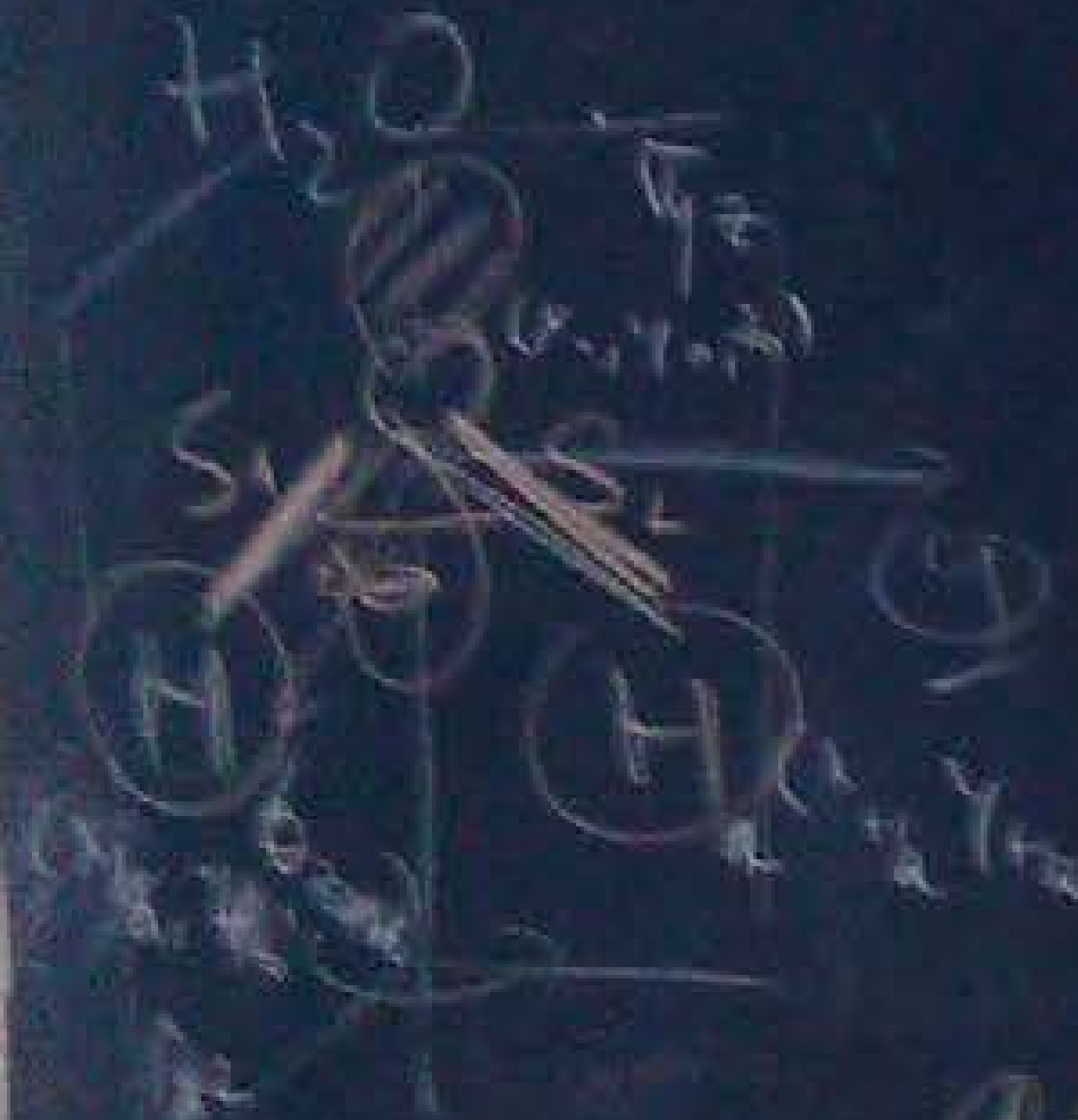
μ
Reprez
"Simbol" de
de Rotatie
a
R_z
x, R_y
y, R_x

sp
Repre
Binare
Blasconi
x², y², z²
xy
xz
yz

Tranducere
→ Rotatie

+ "simbol de grad" de la caracter

simbol de grad de la caracter



1. L. de simetrie
2. L. de simetrie
3. L. de simetrie

$$\Gamma = 2A_1 + B_2$$

IR, Raman (IR + Raman)

Structura și Proprietăți moleculare cu Tabel de Caracteri

$$a_{A_1} = \frac{1}{4} [1 \cdot 1 \cdot 9 + 1 \cdot 1 \cdot (-1) + 1 \cdot 1 \cdot 1 + 1 \cdot 1 \cdot 3]$$

$$a_{A_1} = 3A_1, \quad a_{A_2} = \dots = 1A_2$$

$$a_{B_1} = \frac{1}{4} (5 + 1 + 1 - 3) = 2B_1$$

$$a_{B_2} = 3B_2$$

$$a_i = \frac{1}{h} \sum g \chi(R) \chi(R)$$

$$\Gamma_{tot} = 3A_1 + A_2 + 2B_1 + 3B_2$$

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

Tabel de Caracteri

Numărul de vibrații = 3n - 5 (pentru n=2)

Reprezentare	Reprezentare
"Dipolele" de Rotație	Binare "Rotație"
A_1	x^2, y^2, z^2
A_2	xy
B_1	xz
B_2	yz

$$\Gamma_{\text{vib}} = 2A_1 + B_2$$

IR, Raman (IR+Raman)

Structura și Proprietăți moleculare cu Tabel de Caracter

Repr. în lg. chimic (S_1, S_2)
și unghi diedral (180°)

$$S_1 S_1 = 1, S_2 S_2 = 1, S_1 S_2 = 0 \Rightarrow \Gamma_{\text{vib}} = 2A_1 + B_2$$

cu vibrația
 $N(S_1 S_2)^2 = 1$ S_1 foto de S_2
 $N(S_1 S_2) = 1$ sau vibra. 180° ?

? descrierea modurilor
de vibr. Moleculare
(în ansamblul ei) pe molecule

(+) Metoda
a proiectiei
diferențiale
pe axa de simetrie

A_1, A_2, B_1, B_2

Prin urmare

$$\Gamma_{A_1}(S_1) = \frac{1}{4} (1 \cdot E(S_1) + 1 \cdot C_2(S_1) + 1 \cdot \sigma_{xz}(S_1) + 1 \cdot \sigma_{yz}(S_1))$$

$$\Gamma_{B_2}(S_1) = \frac{1}{4} (1 \cdot S_1 - S_2 - S_2 + S_1) = \frac{1}{2} (S_1 - S_2)$$

$$P(A_1) = \frac{1}{4} (1 \cdot 180 + 1 \cdot 180 + 1 \cdot 180 + 1 \cdot 180) = 180$$

C_{2v}	E	C_2	σ_{xz}	σ_{yz}	Repr. 2 "Displacement" de Rotatie	Repr. Binare "Displacement"
A_1	1	1	1	1	$\frac{1}{2} \frac{1}{2}$	x^2, y^2, z^2 $-1/1$
A_2	1	1	-1	-1	$\frac{1}{2} \frac{1}{2}$	xy
B_1	1	-1	1	-1	$\frac{1}{2} \frac{1}{2}$	xz
B_2	1	-1	-1	1	$\frac{1}{2} \frac{1}{2}$	yz

Translație

Rotatie

+ "moduri de vibrație" ale moleculei

moduri de vibrație
moleculare
IR, Raman

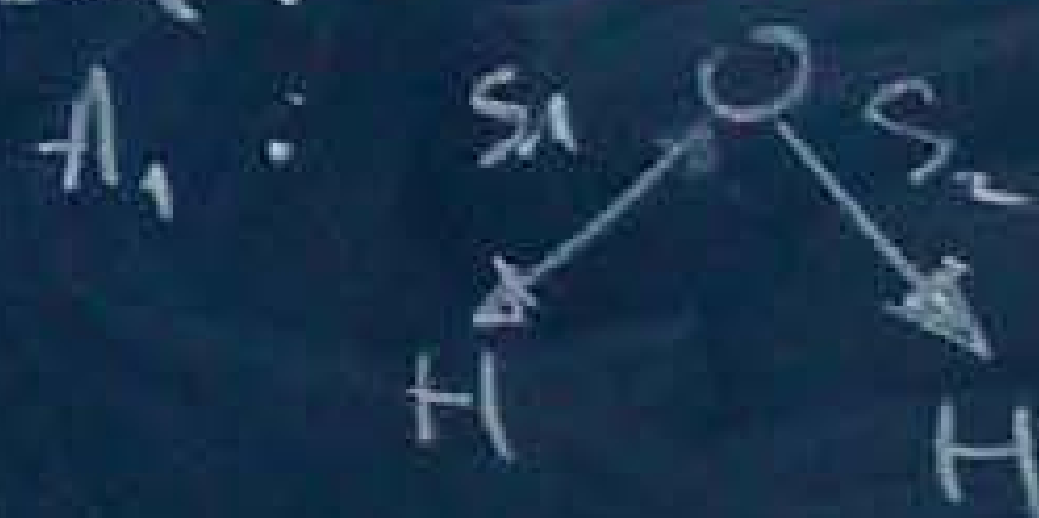
$$\Gamma = 2A_1 + B_2$$

IR, Raman (IR + Raman)

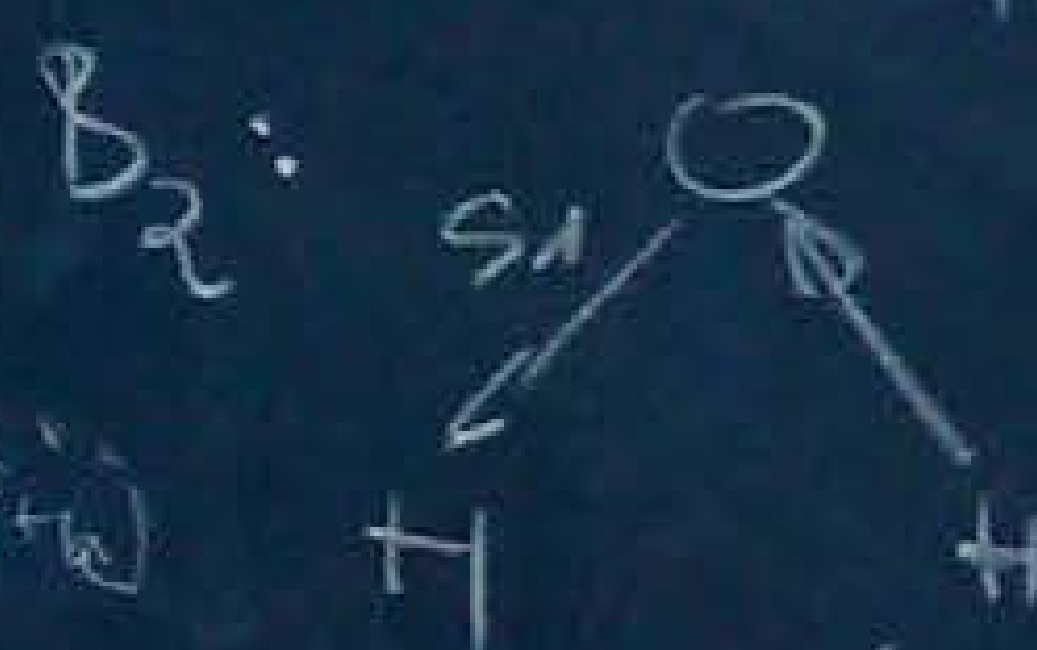
Structura și Proprietăți moleculare cu Tolu de Cărbune

Modurile de Vibrație

Sunt:



(Symmetrical stretching)



(Symmetrical anti-stretching)



(bending)

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

$$P_{H_2O} = \frac{1}{4} (1 + 1 + 1 + 1) = 1$$

Repr. "Dipole" in de Rădăre

Repr. "Dipole" in de Rădăre

Repr. "Dipole" in de Rădăre	Repr. "Dipole" in de Rădăre
A_1	x^2, y^2, z^2
A_2	xy
B_1	xz
B_2	yz

(+) Metoda a proiectiei

Proiecții

$$P_{A_1}(S_1) = \frac{1}{4} (1 \cdot \hat{E}(S_1) + 1 \cdot \hat{C}_2(S_1) + 1 \cdot \hat{\sigma}_{xz}(S_1) + 1 \cdot \hat{\sigma}_{yz}(S_1)) = \frac{1}{4} (S_1 + S_2 + S_1 + S_1) = \frac{1}{4} (3S_1 + S_2)$$

$$P_{A_2}(S_1) = \frac{1}{4} (1 \cdot \hat{E}(S_1) + 1 \cdot \hat{C}_2(S_1) - 1 \cdot \hat{\sigma}_{xz}(S_1) - 1 \cdot \hat{\sigma}_{yz}(S_1)) = \frac{1}{4} (S_1 + S_2 - S_1 - S_1) = \frac{1}{4} (-S_1 + S_2)$$

Translație

Rotatie

Modurile de vibrație

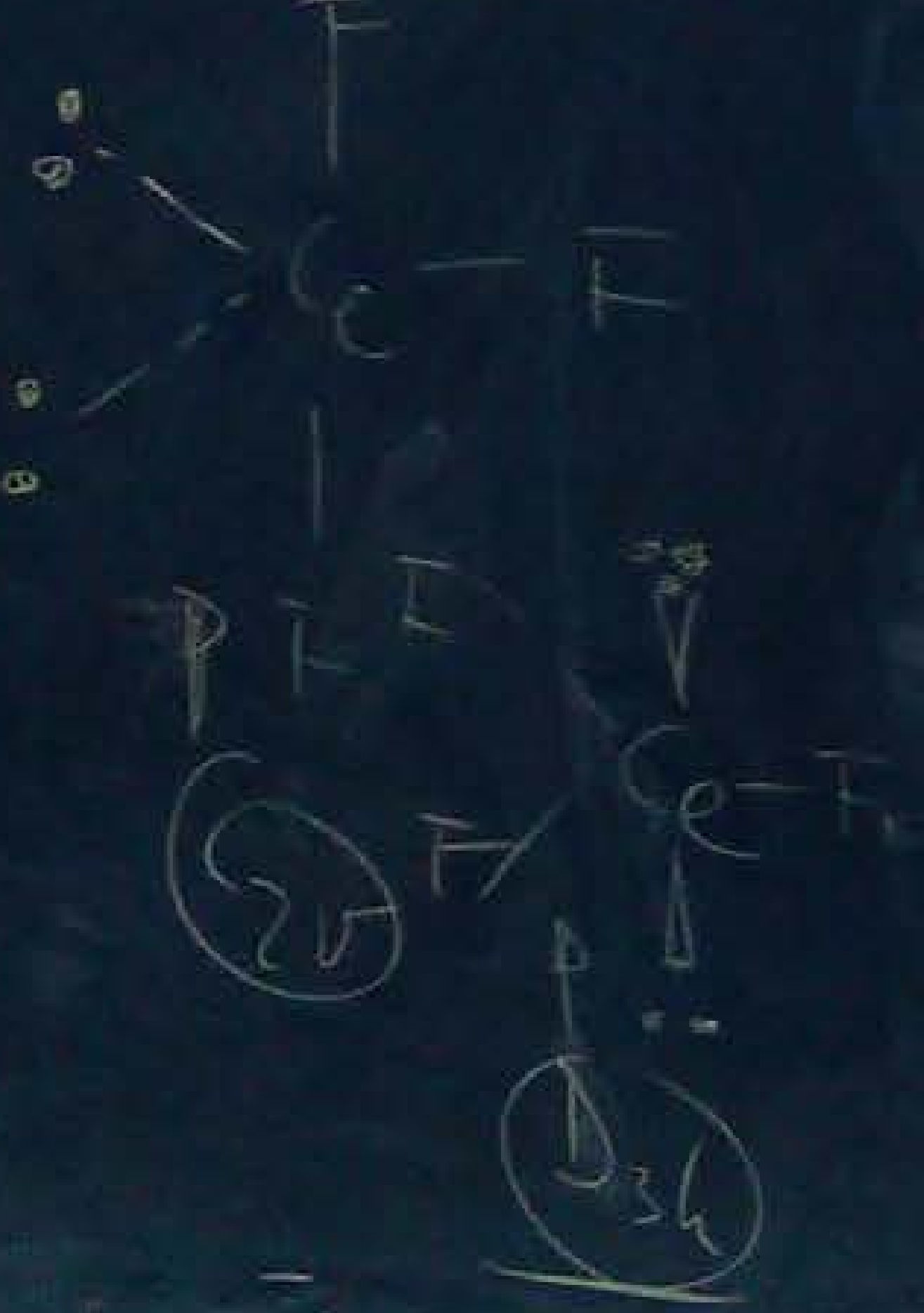
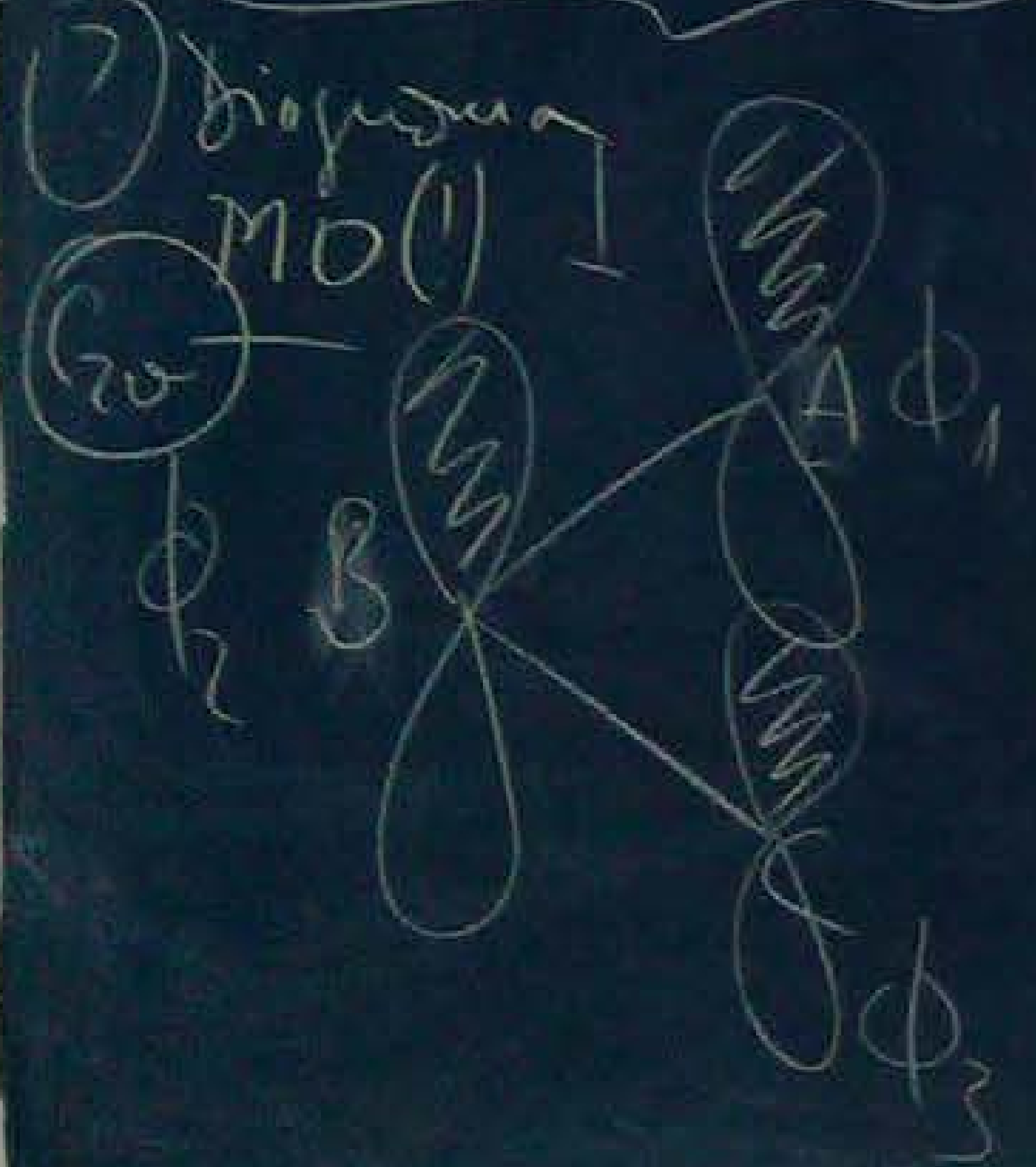
$$\Gamma_{\text{vib}} = 2A_1 + B_2$$

IR, Raman (IR + Raman)

Structure et Propriétés moléculaires en Tolu de Casacese

$$P(\text{MO}) = \frac{1}{4} (100 + 100 + 100 + 100) = 100$$

NO_2^- , C_3H_5 , ClF_3 (T-slope)

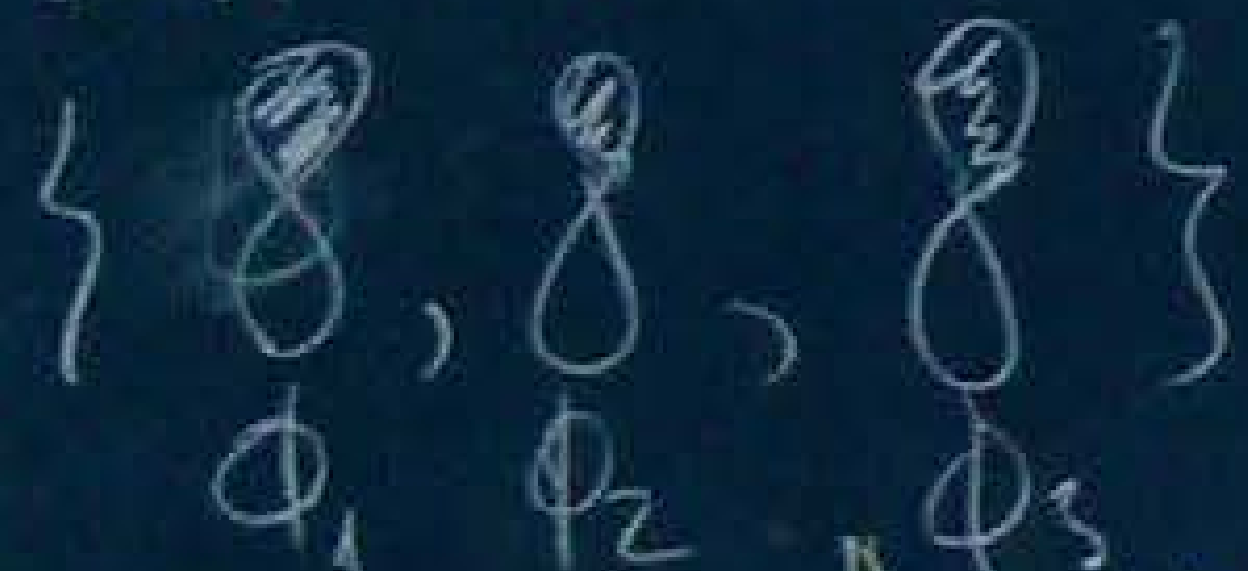


	C_{2v}	E	C_2	σ_{xz}	σ_{yz}	Représ. "Dipolaires" de Rot. de Rot. de Rot.	Représ. "p" Binaires "Binaires"
A_1	1	1	1	1	1	$\hat{z}$	x^2, y^2, z^2
A_2	1	1	1	-1	-1	R_z	xy
B_1	1	-1	1	1	-1	x, R_y	xz
B_2	1	-1	1	-1	1	y, R_x	yz

+ "mouvement de queue" de la molécule

mouvement de la molécule

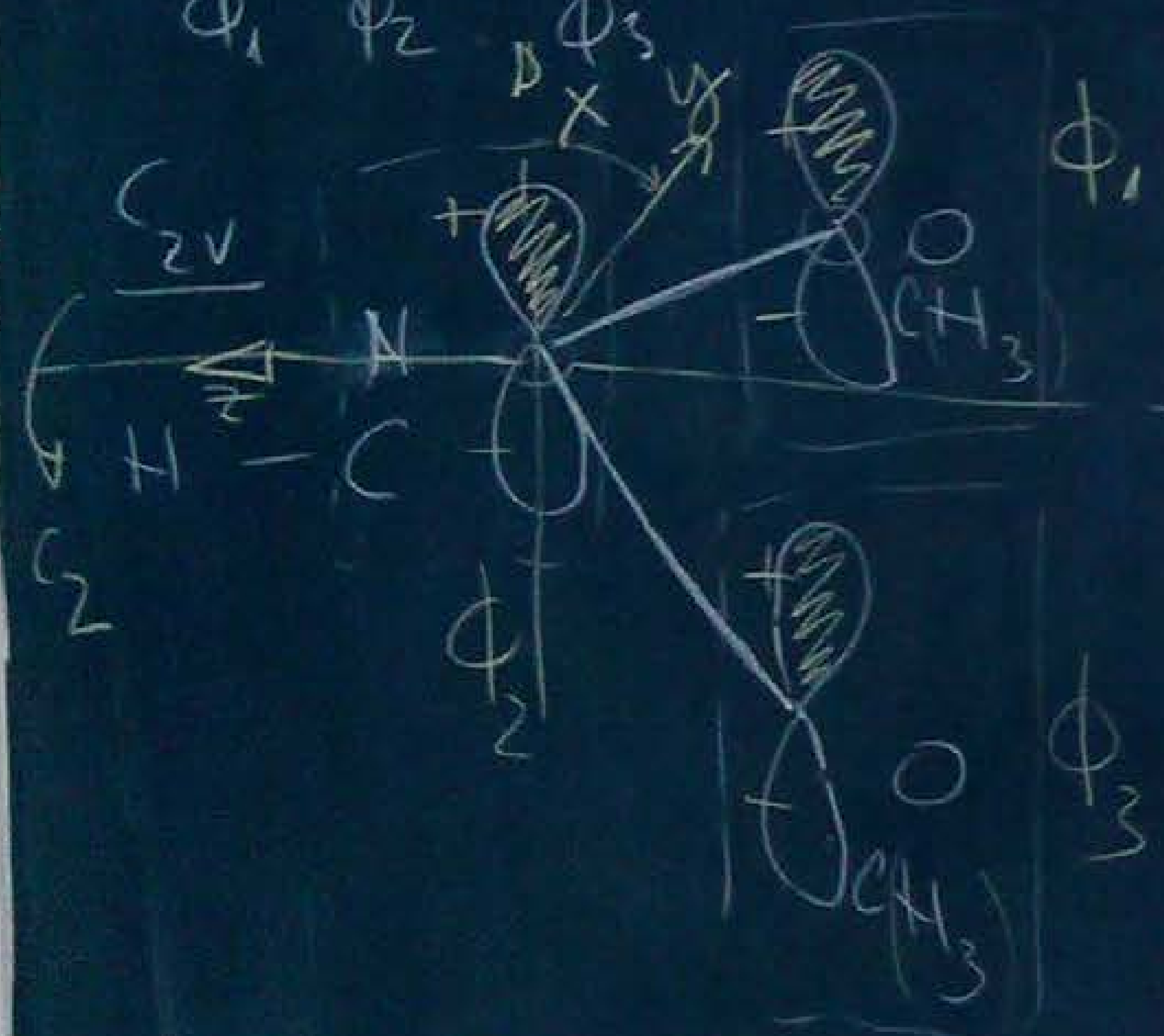
Baza orbitalo



Metoda "SALC" și Hückel

Symmetry Adopted Linear Combination

Quantum Symmetry



C_{2v}	E	C_2	σ_{xz}	σ_{yz}
Γ_ϕ	3×1	$1(-1)$	$1(1)$	$3(-1)$
Γ_ϕ	3	-1	1	-3

Reducere
pe
Componente
irreductibile
(2)

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

"Orbital
molecular
global"

$$\Gamma_\phi = \Gamma_\phi(A_2, 2B_1)$$

SALC ($d\phi$)

I) ? Sym. Irreductibile specifice lui Γ_ϕ ?

$$a_{A_1} = \frac{1}{4} (1 \cdot 3 + 1(-1)1 + 1(1)1 + 1(-3)1) = 0 A_1$$

$$a_{A_2} = \frac{1}{4} (1 \cdot 3 - 1 \cdot 1 + 1(-1)1 - 1(1)1) = 1 A_2$$

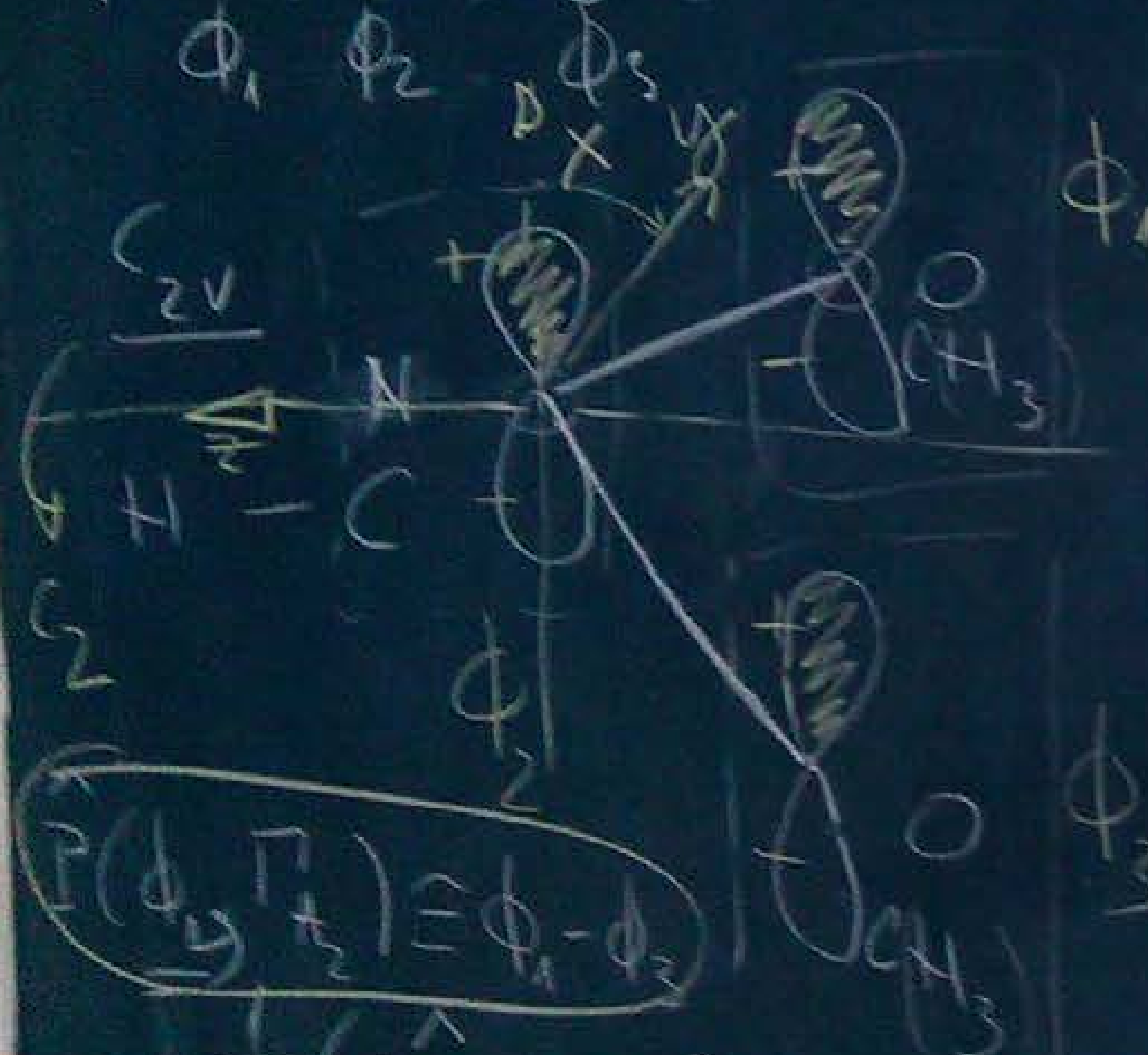
$$a_{B_1} = \frac{1}{4} (8) = 2 B_1$$

$$a_{B_2} = \frac{1}{4} (0) = 0 B_2$$

Metoda "SALC" i Hückel

Symmetry Adapted Linear Combination

Baza atomowa



Quantum Symmetry Representation 3x3

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
Γ_ϕ	3×1	$1(-1)$	$1(1)$	$3(-1)$
1	3	-1	1	-3

Reducere
na
compone
irreducibile
(?)

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

"orbitale lokalne global"

$$\Gamma_\phi = \Gamma_\phi (A_2, 2B_1)$$

Procedura tworzenia

Próba do ko OA $\rightarrow$ OM

$$P(\phi_1, \Gamma_{B_1}) = \frac{1}{4} (1\phi_1 - 1\phi_2 + 1\phi_3 - 1\phi_4)$$

$$P(\phi_2, \Gamma_{B_2}) = \frac{1}{4} (1\phi_1 - 1\phi_2 - 1\phi_3 + 1\phi_4)$$

$$(\phi_1, \phi_2, \phi_3) = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 \end{pmatrix}$$

$$P(\phi_1, \Gamma_{B_1}) = \frac{1}{4} (1\phi_1 - 1\phi_2 + 1\phi_3 - 1\phi_4)$$

$$P(\phi_2, \Gamma_{B_2}) = \frac{1}{4} (1\phi_1 - 1\phi_2 - 1\phi_3 + 1\phi_4)$$

$$P(\phi_1, \Gamma_{A_2}) = \phi_1 - \phi_3$$

$$\frac{1}{4} (1\phi_1 + 1\phi_2 + 1\phi_3 + 1\phi_4) \sim \phi_1 + \phi_2$$

Base atoms



Metoda "SALC" pi Hückel

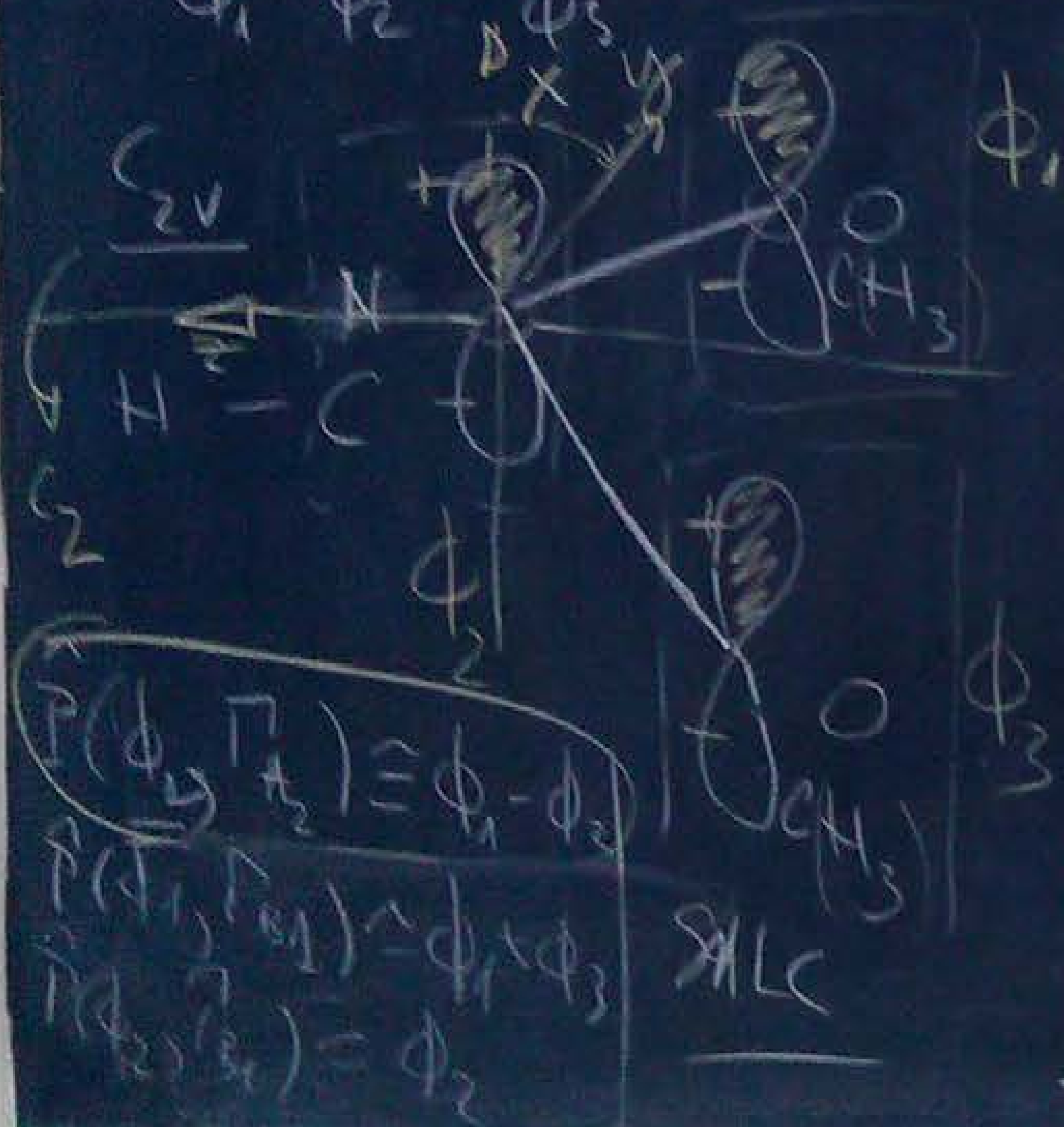
Symmetry Adapted Linear Combination

? Energie of MO Proper?

Quantum Superposition

$$\hat{H} \psi_{MO} = E_{MO} \psi_{MO}$$

$$\psi_{MO} = \sum_{i=1}^n c_{ik} \phi_i^{OA}$$



"Orbital Molecular Orbital"

$$(\hat{H} - E_{MO}) \psi_{MO} = 0$$

integrate (Integral of function)

$$\int \sum_k c_k \phi_k (\hat{H} - E_{MO}) \sum_l c_l \phi_l d\tau = 0$$

$$\psi = c_1 \phi_1^{OA} + c_2 \phi_2^{OA} + c_3 \phi_3^{OA}$$

$k = \text{end of SALCs}$

$$\int \phi_i \hat{H} \phi_j d\tau = H_{ij}$$

$$\int \phi_i \phi_j d\tau = \delta_{ij}$$

Basis orbitale

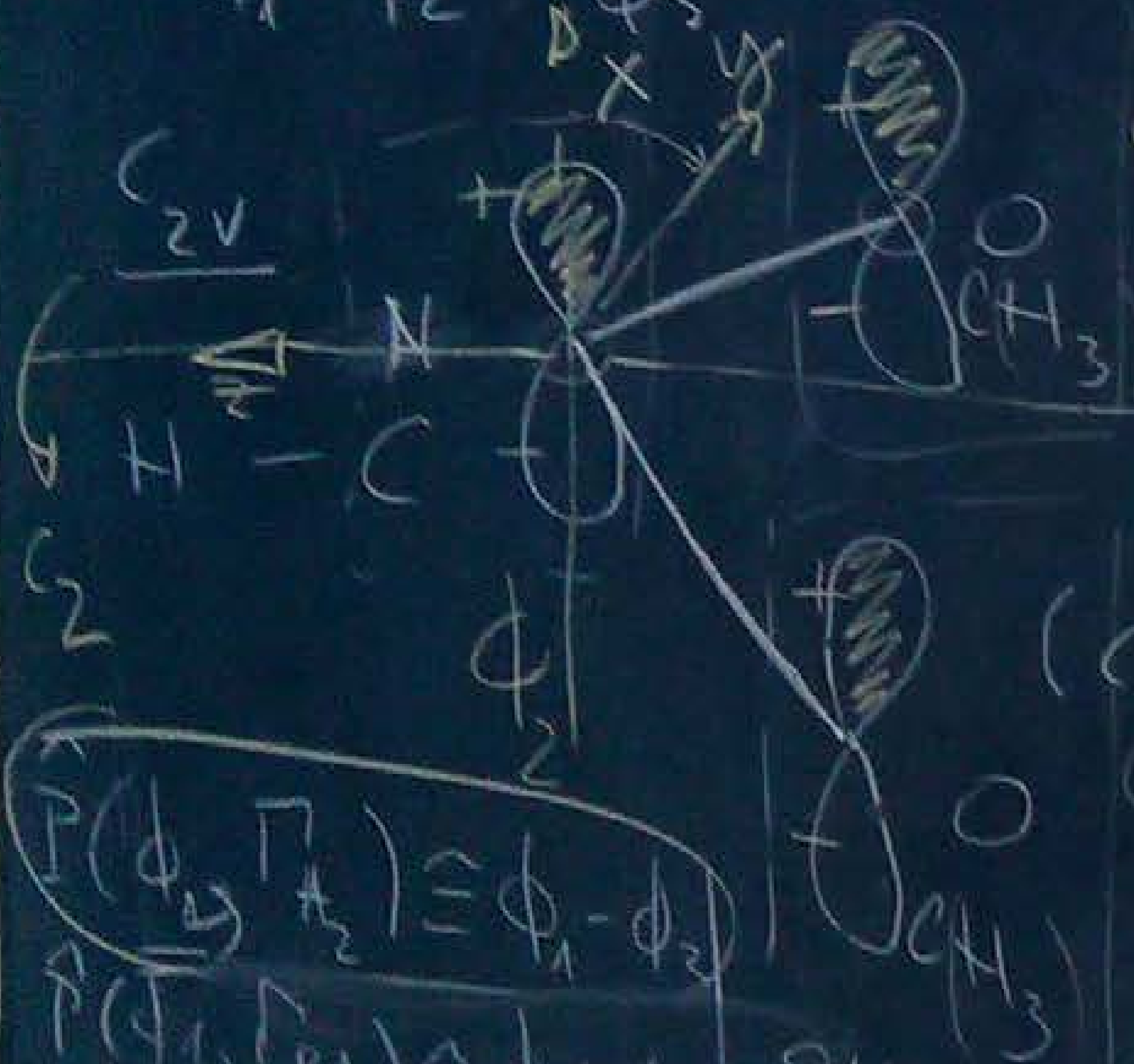
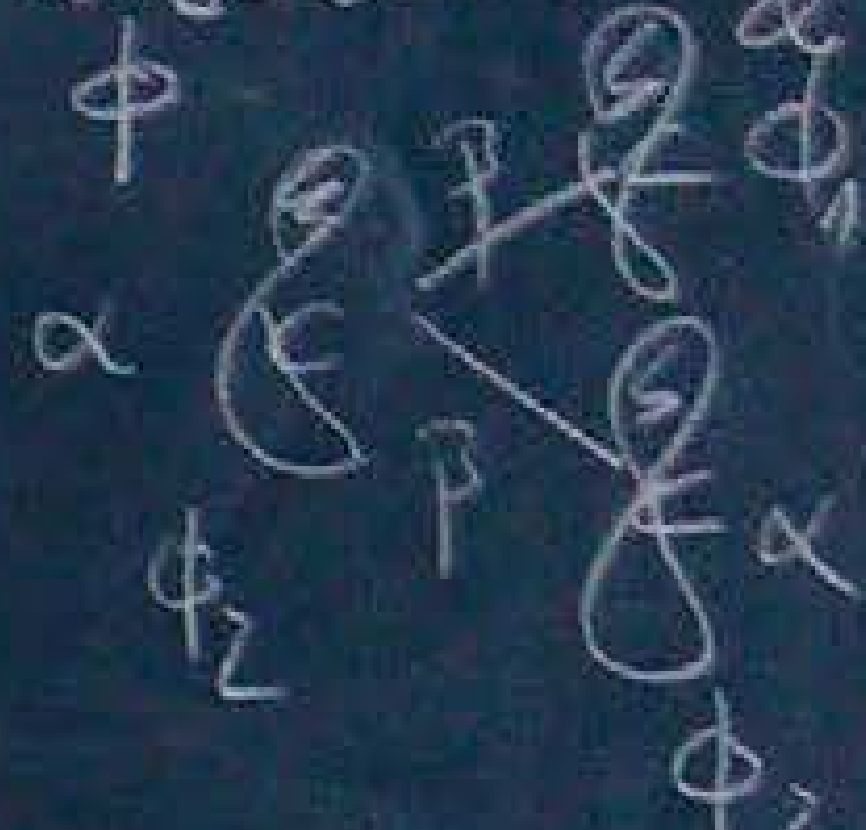


Metoda "SALC" și Hückel

Approximativă Hückel (combinații) ← Graf → Grafuri / Schimbări
at. de carbon cu
sau ϕ

Hückel 1): tot α , sunt egali $\Rightarrow \boxed{3! \alpha}$

Hückel 2): tot $\beta_{i,j} = \beta \neq 0$



$P(\phi_1, \phi_2) = \phi_1 - \phi_2$
 $P(\phi_1, \phi_3) = \phi_1 + \phi_3$
 $P(\phi_2, \phi_3) = \phi_2$

SALC

	ϕ_1	ϕ_2	ϕ_3
ϕ_1	$\alpha - E_0$	β	0
ϕ_2	β	$\alpha - E_0$	β
ϕ_3	0	β	$\alpha - E_0$

$\sum_k C_k \phi_k (H - E_0) \sum_k C_k \phi_k = 0$

$\begin{pmatrix} C_{1K} \\ C_{2K} \\ C_{3K} \end{pmatrix}$

$= 0$

$\Rightarrow \begin{vmatrix} \alpha - E_0 & \beta & 0 \\ \beta & \alpha - E_0 & \beta \\ 0 & \beta & \alpha - E_0 \end{vmatrix} = 0$

$\int \phi_i \hat{H} \phi_i d\tau = \alpha_i$

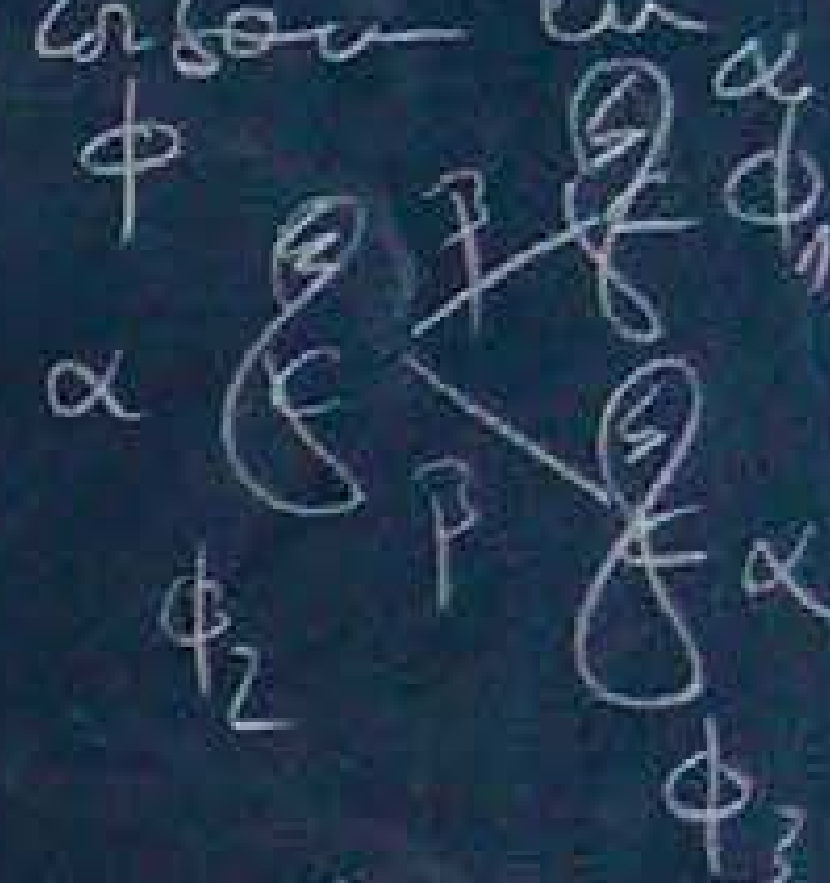
$\int \phi_i \hat{H} \phi_j d\tau = \beta_{ij}$

$\int \phi_i \phi_j d\tau = \begin{cases} 1, & i=j \\ 0, & i \neq j \end{cases} = \delta_{ij}$

Metoda "SALC" i Hückel

Approximativ Hückel (Carbonhidrat)

Graf → Graf / Schicht
 ut. de carbon en
 5-2-φ



$$\begin{matrix} \phi_1 & \phi_2 & \phi_3 \\ \left\{ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \right\} & x=0 \\ \left\{ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \right\} & x=+\sqrt{2} \\ \left\{ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \right\} & x=-\sqrt{2} \end{matrix}$$

$$X = \frac{\alpha - E}{\beta} \Rightarrow \begin{vmatrix} X & 1 & 0 \\ 1 & X & 1 \\ 0 & 1 & X \end{vmatrix} = 0$$

získati

$$x^3 - 2x = 0 \Rightarrow x = \{0, +\sqrt{2}, -\sqrt{2}\}$$

$$E = \left\{ \alpha, \alpha - \sqrt{2}\beta, \alpha + \sqrt{2}\beta \right\}$$

$$\Rightarrow \begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} = 0$$

$$\beta = <0| \quad E = \alpha \pm \beta$$

α-βep
 $\psi_{no3} = \frac{1}{2}\phi_1 - \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$

α-βep
 $\psi_{no2} = \frac{1}{\sqrt{2}}\phi_1 = \frac{1}{\sqrt{2}}\phi_3$

α+βep
 $\psi_{no1} = \frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$

$$\psi_k = c_{1k}\phi_1 + c_{2k}\phi_2 + c_{3k}\phi_3 \quad k=1,2,3$$

$$\begin{vmatrix} X & 1 & 0 \\ 1 & X & 1 \\ 0 & 1 & X \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0$$

$$\begin{cases} c_1 X + c_2 = 0 \\ c_1 + c_2 X + c_3 = 0 \\ c_2 + c_3 X = 0 \end{cases}$$

$$\sum_k c_k^2 = 1 \Rightarrow c_1^2 + c_2^2 + c_3^2 = 1$$

✓ Omul este măsurat
 tuturor lucrurilor!

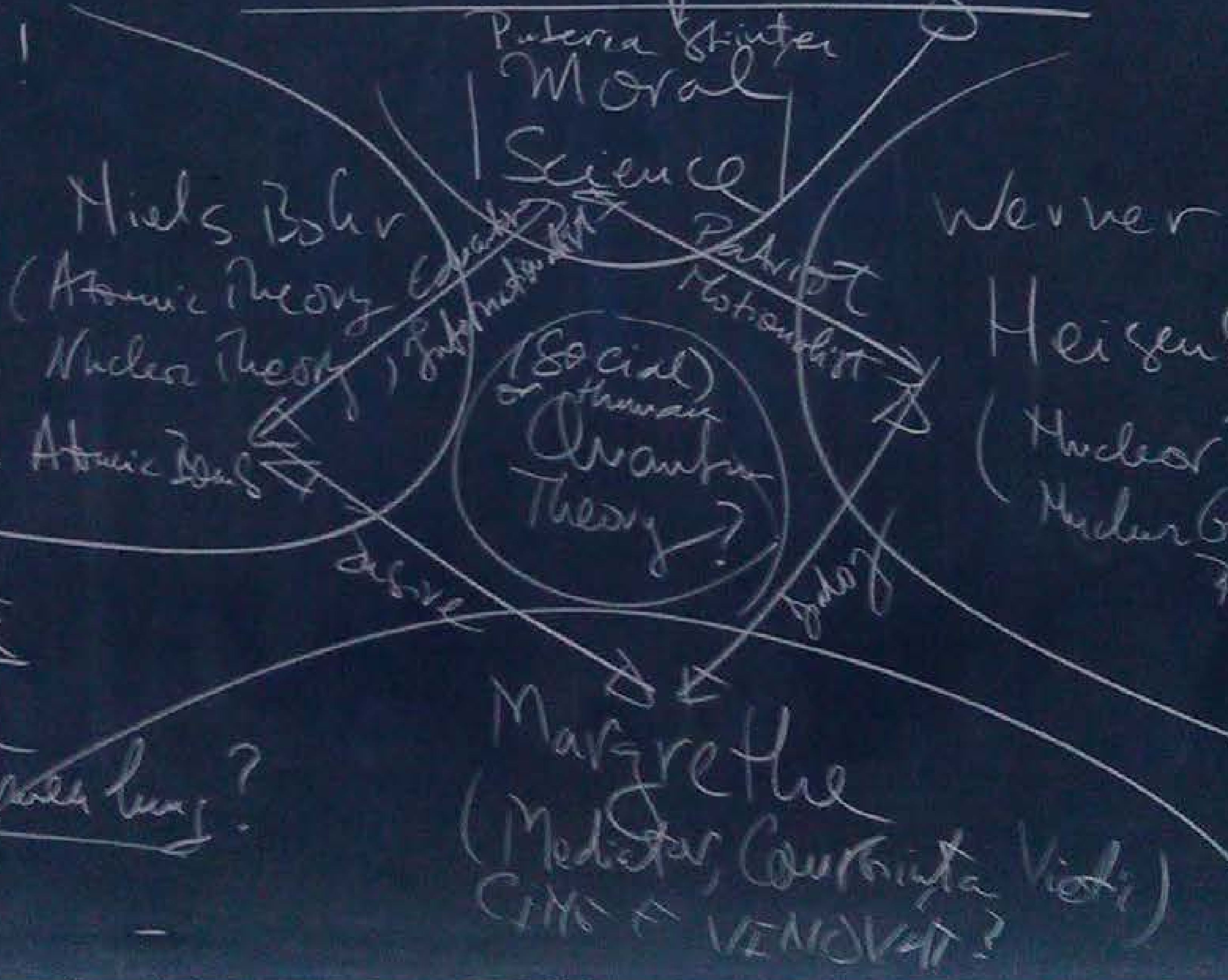
(~ Protagoras)

✓ Are dreptul moral
 un om de știință să
 pună în aplicare
 descoperirile sa

Donc Atomic War

Chiar cu condiția
 unui război în Germania
 Indestructibilă la nivel
 uman și etic, pe termen lung?

Copenhagen



$$\nabla \cdot \vec{E} = + i \hbar \frac{\partial}{\partial t} \psi$$

de la prima
 y la derivata
 Vacuum a v. difer.

12x nihilo

Vacuum

$$\vec{p} \cdot = - i \hbar \frac{\partial}{\partial x}$$

