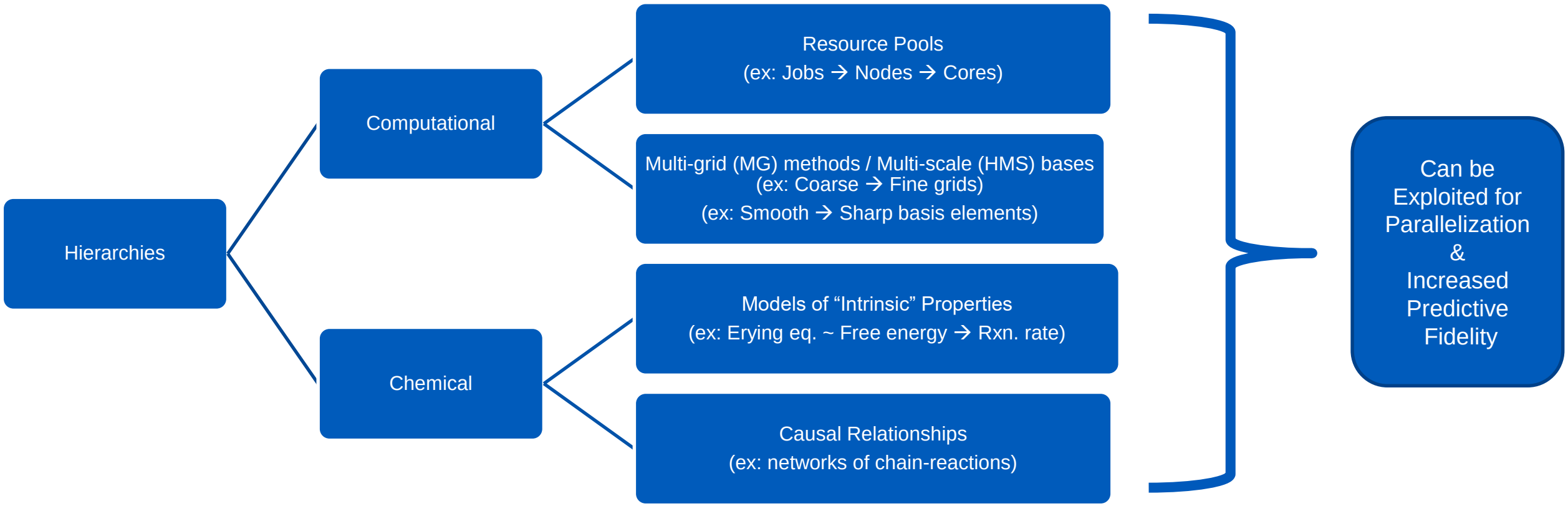
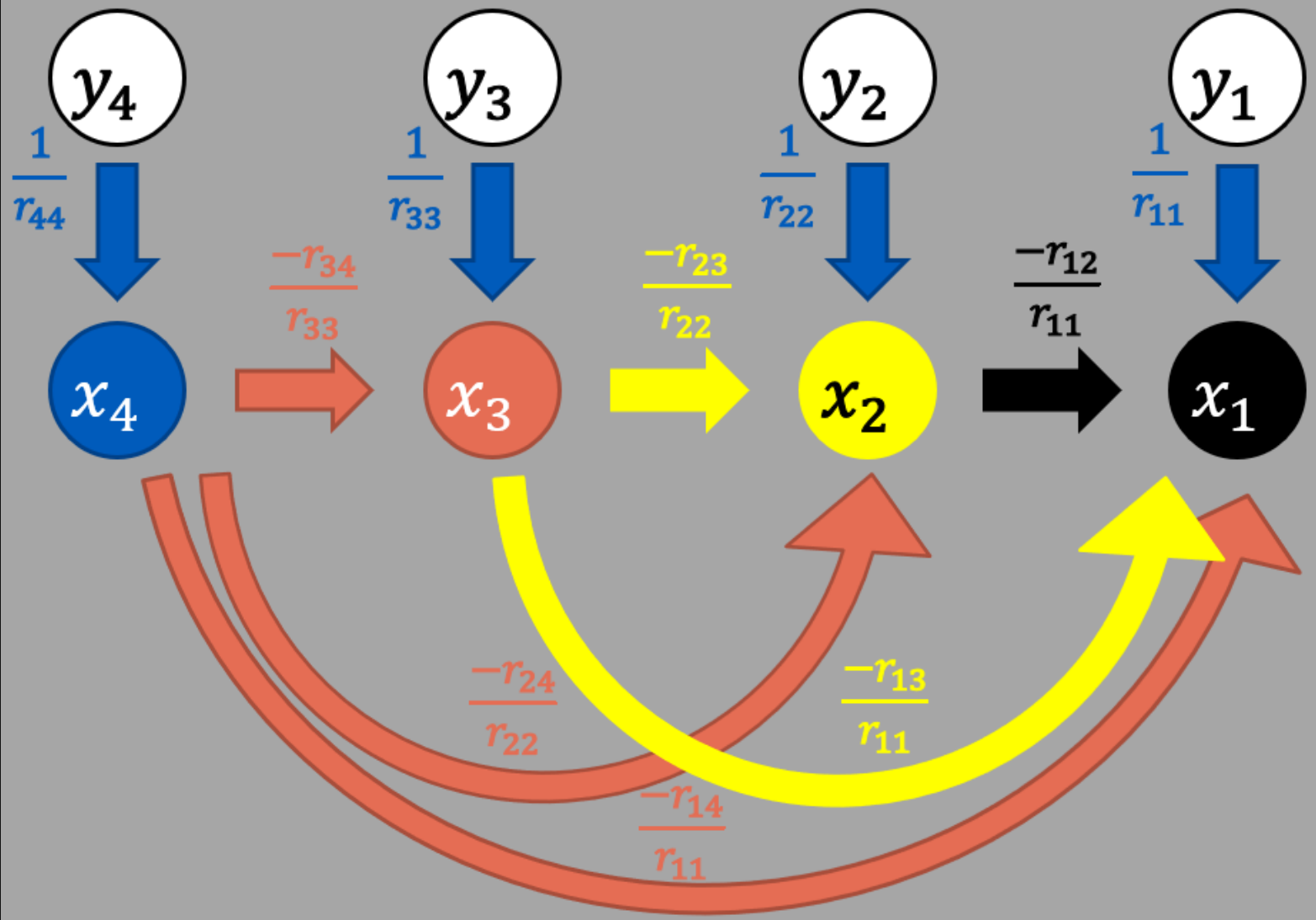
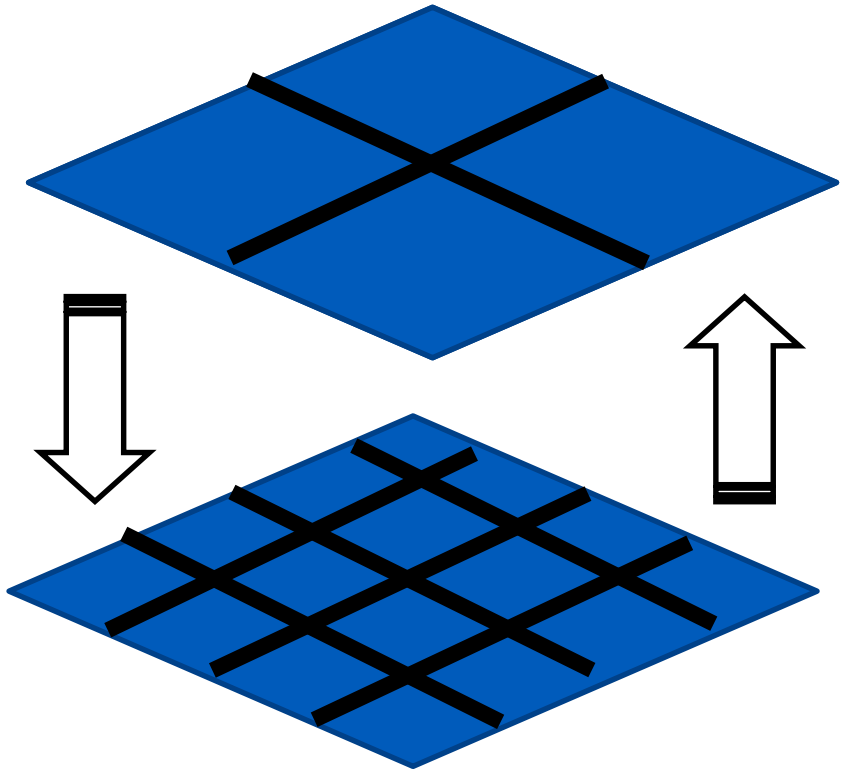

Hierarchies
Computational
Chemical
Resource Pools
(ex: Jobs → Nodes → Cores)
Multi-grid (MG) methods / Multi-scale (HMS) bases
(ex: Coarse → Fine grids)
(ex: Smooth → Sharp basis elements)
Models of “Intrinsic” Properties
(ex: Erying eq. ~ Free energy → Rxn. rate)
Causal Relationships
(ex: networks of chain-reactions)
Can be Exploited for Parallelization & Increased Predictive Fidelity

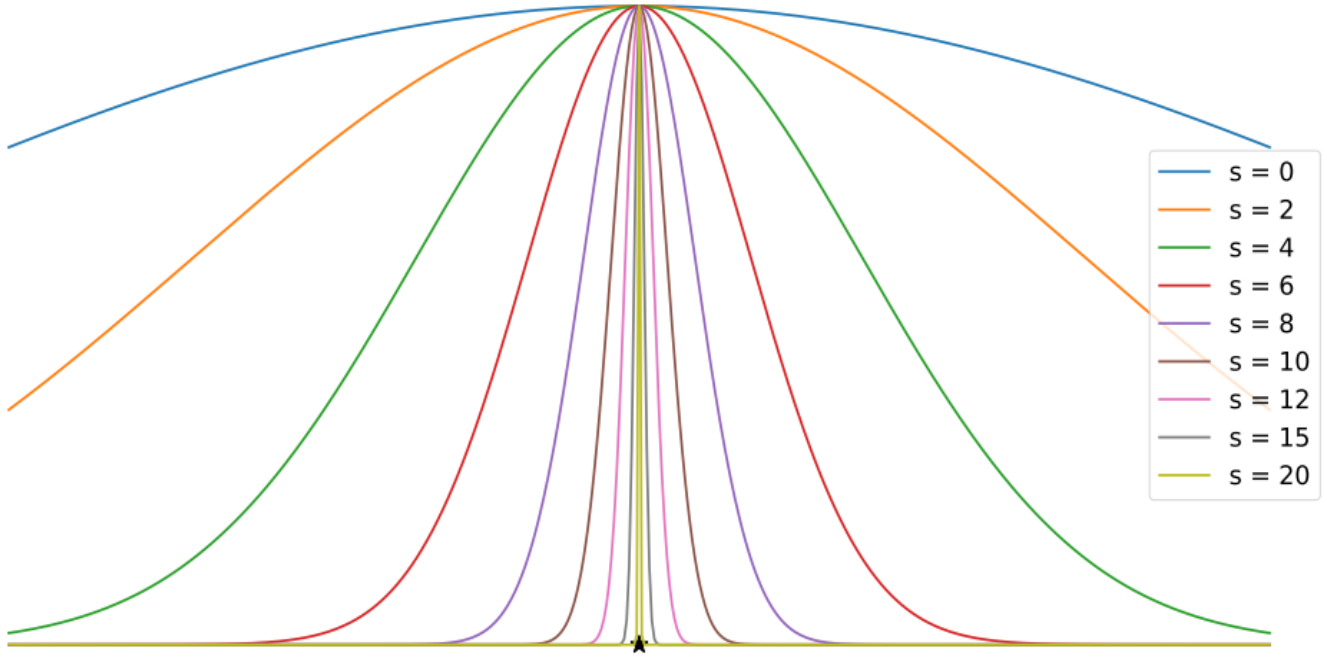
i = sample index
j = row index
k = column index

$$x_{i,j} = \frac{1}{r_{i,jj}}\left(y_{i,j} - \sum_{k=j+1}^{m} r_{i,jk}x_{i,k}\right)$$

on node i do:
  on proc j do:
    x[i][j] = y[i][j]/R[i][j, j] # bcast update
    for k in range(N-j):
      x[i][j] =- R[i][j, N-k]*x[i][N-k] /R[i][j, j]
      # bcast updates






s = 0
s = 2
s = 4
s = 6
s = 8
s = 10
s = 12
s = 15
s = 20

$$U = -\left(\frac{\partial}{\partial\beta}\ln Q\right)_V = -N\left(\left(\frac{\partial}{\partial\beta}\ln q_T\right)_V + \left(\frac{\partial}{\partial\beta}\ln q_R\right)_V + \left(\frac{\partial}{\partial\beta}\ln q_V\right)_V + \left(\frac{\partial}{\partial\beta}\ln q_E\right)_V\right)$$

$$U_T = \frac{3}{2}Nk_BT = \text{3D Translational internal energy}$$

$$U_R = \text{Rotational internal energy} = \begin{cases} Nk_BT & \text{diatomic and linear polyatomic} \\ \frac{3}{2}Nk_BT & \text{nonlinear polyatomic} \end{cases}$$

$$U_V = \frac{Nhc\tilde{\nu}}{e^{\beta hc\tilde{\nu}} - 1} = \text{Vibrational internal energy neglecting ZPE}$$

$$U_E = 0 = \text{Electronic internal energy for ground} - \text{state degeneracy}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = -k_B\beta^2\left(\frac{\partial U}{\partial \beta}\right)_V = \text{Heat capacity at constant volume}$$

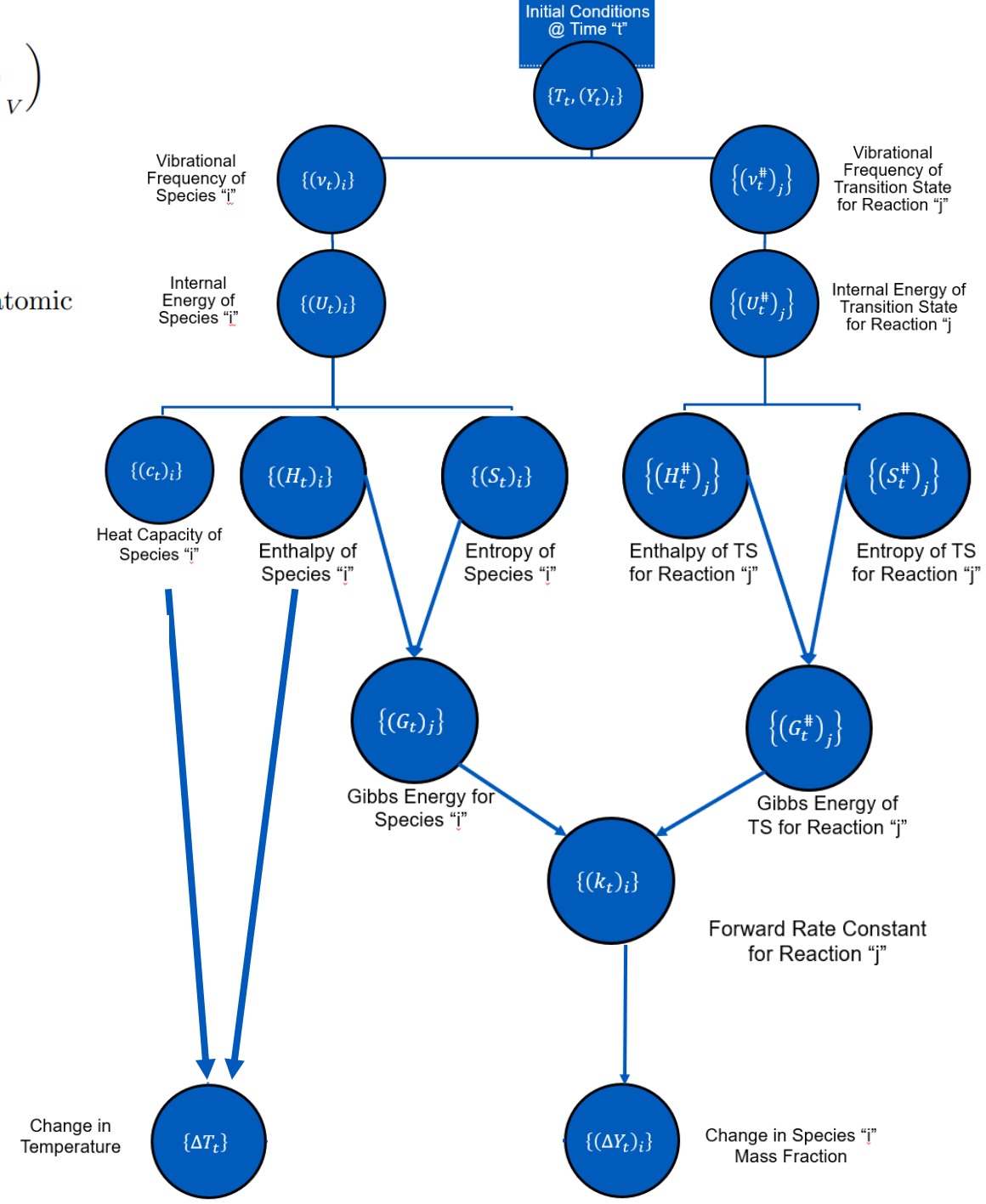
$$S = \frac{U}{T} + k_B\ln Q = \text{Entropy}, \qquad H = U + PV = \text{Enthalpy}$$

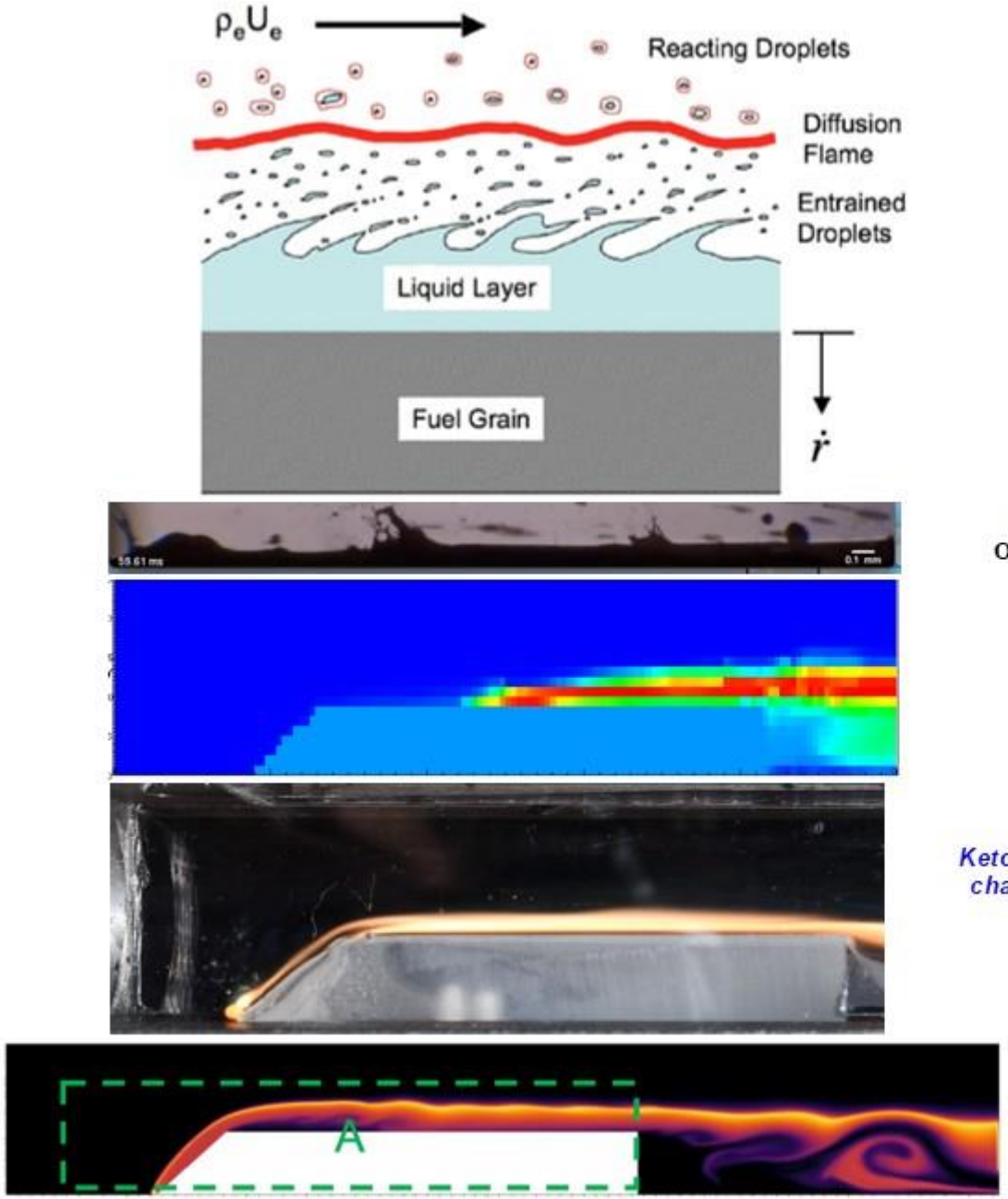
$$\Delta G = \Delta H - T\Delta S = \text{Gibbs free energy of reaction}$$

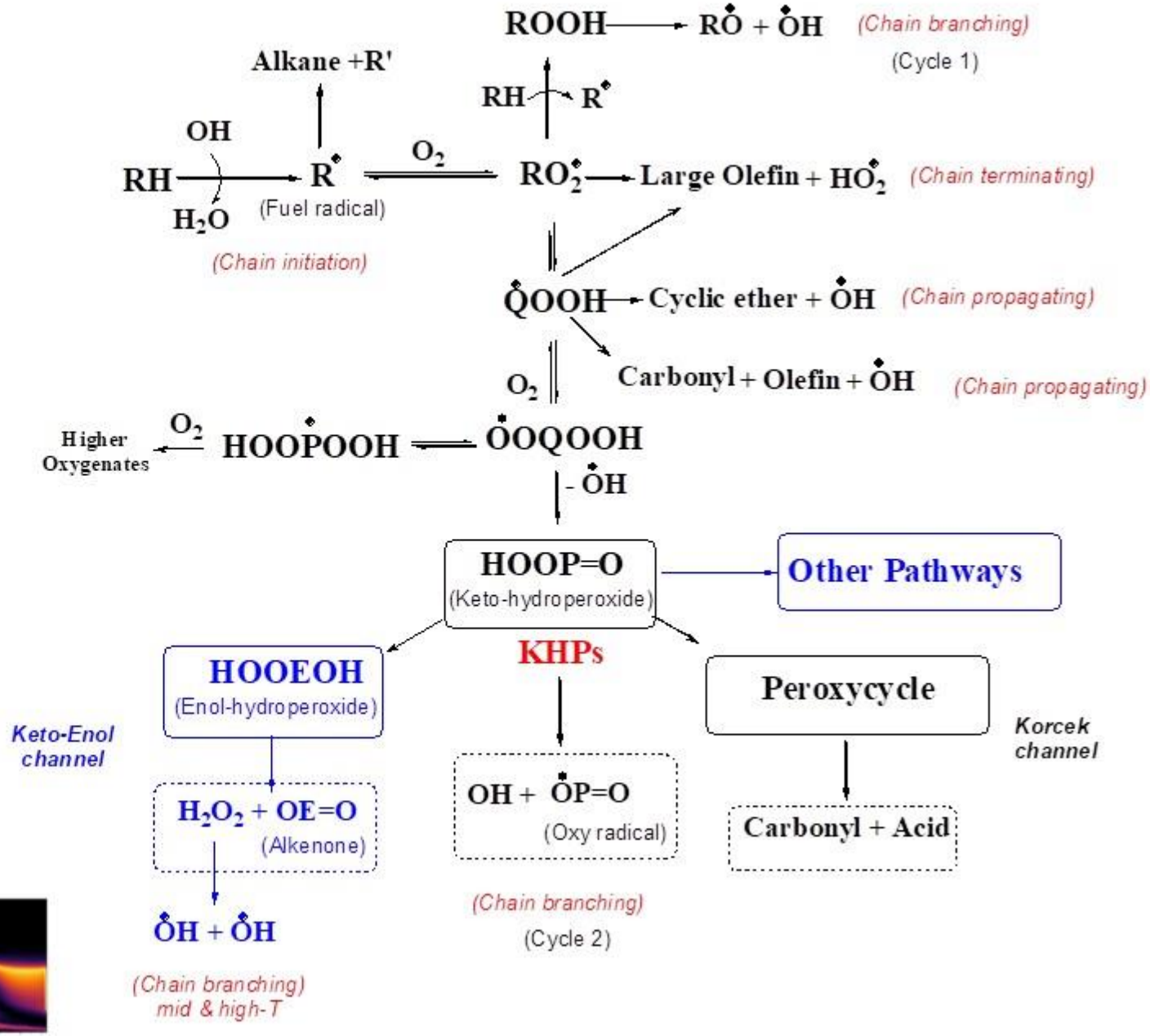
$$\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger} = \text{Gibbs free energy of activation}$$

$$k_f = \frac{k_bT}{h}\exp\left(-\frac{\Delta G^{\ddagger}}{k_bT}\right), \qquad k_r = \frac{k_f}{K}, \qquad K = \exp\left(\frac{\Delta G}{k_bT}\right),$$

$$k_f = AT^b\exp\left(-\frac{E_a}{RT}\right),$$




$\rho_e U_e$
Reacting Droplets
Diffusion Flame
Entrained Droplets
Liquid Layer
Fuel Grain
$\dot{r}$
A


ROOH → RȮ + ȮH (Chain branching)
(Cycle 1)
Alkane +R'
RH
R•
OH
RH → R• → H2O
(Fuel radical)
(Chain initiation)
O2
RO2• → Large Olefin + HO2• (Chain terminating)
Q̇OOH → Cyclic ether + ȮH (Chain propagating)
O2
Carbonyl + Olefin + ȮH (Chain propagating)
Higher Oxygenates
O2
HOOPOOH
ȮOQOOH
- ȮH
HOOP=O
(Keto-hydroperoxide)
Other Pathways
KHPs
HOOEOH
(Enol-hydroperoxide)
Peroxycycle
Keto-Enol channel
Korcek channel
H2O2 + OE=O
(Alkenone)
OH + ȮP=O
(Oxy radical)
Carbonyl + Acid
ȮH + ȮH
(Chain branching)
mid & high-T
(Chain branching)
(Cycle 2)

Solid
Indivisible
Sphere

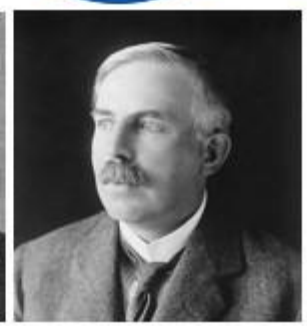
Electron
Plum
Pudding

Dense
Positive
Nucleus

"Bohr
-bits"

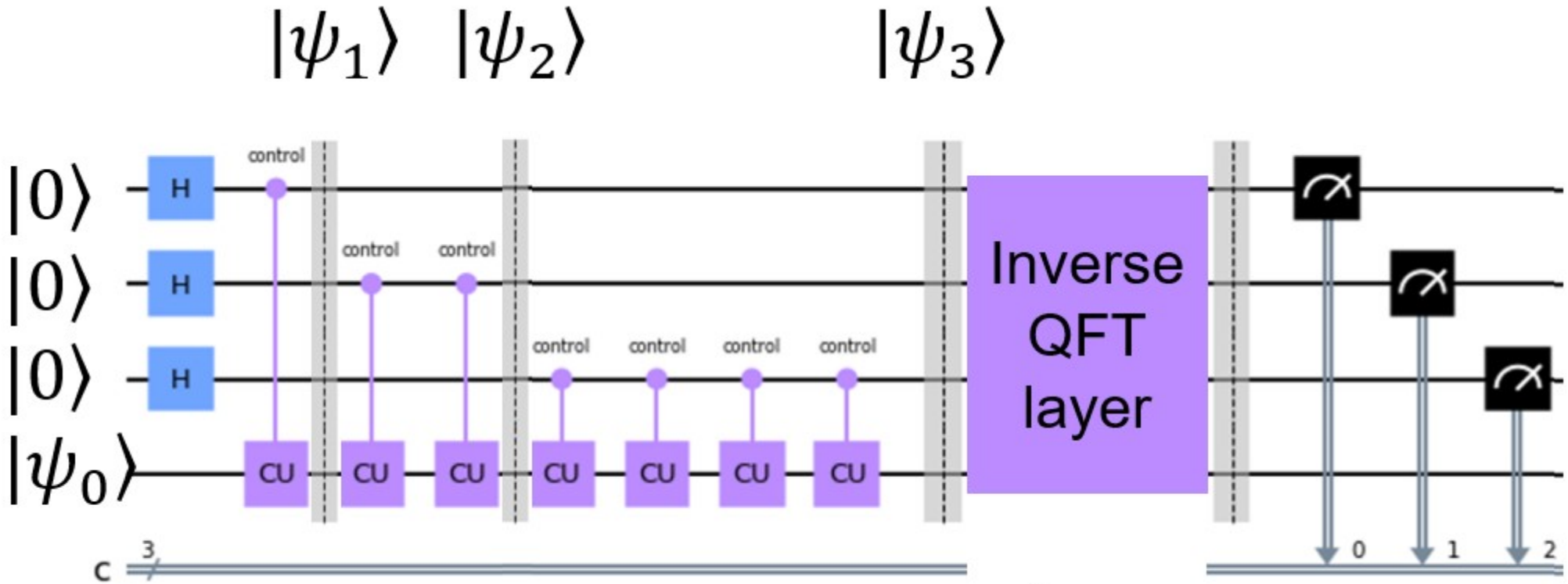
Wave
Mechanics



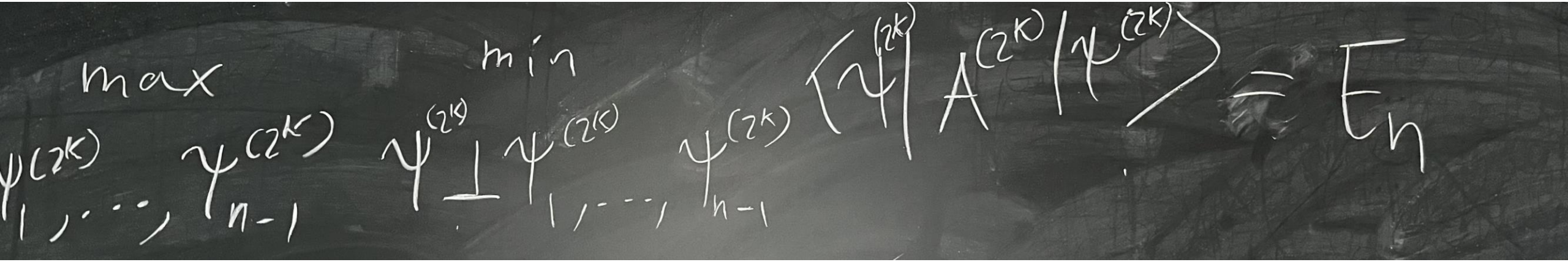


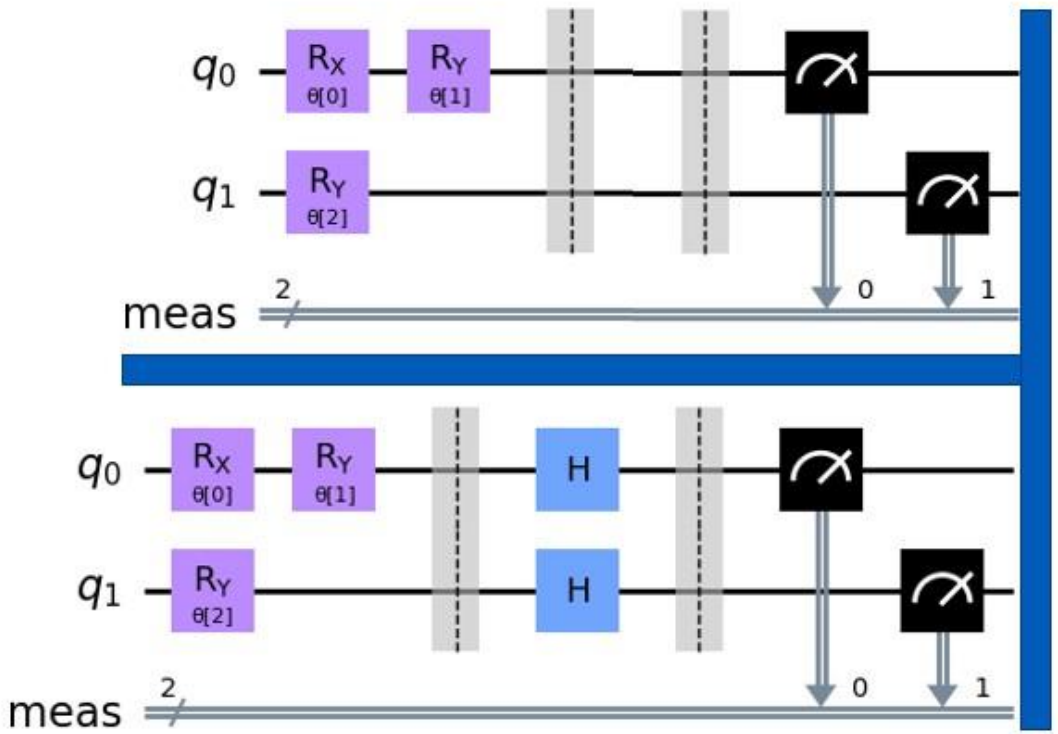
Dalton **T**homson **R**utherford **B**ohr **S**chrodinger

Don't Take Ricky Bobby's Shoes



QPE **almost** like: $|\psi_{k+1}\rangle = \boldsymbol{U^{2^k}}|\psi_k\rangle$

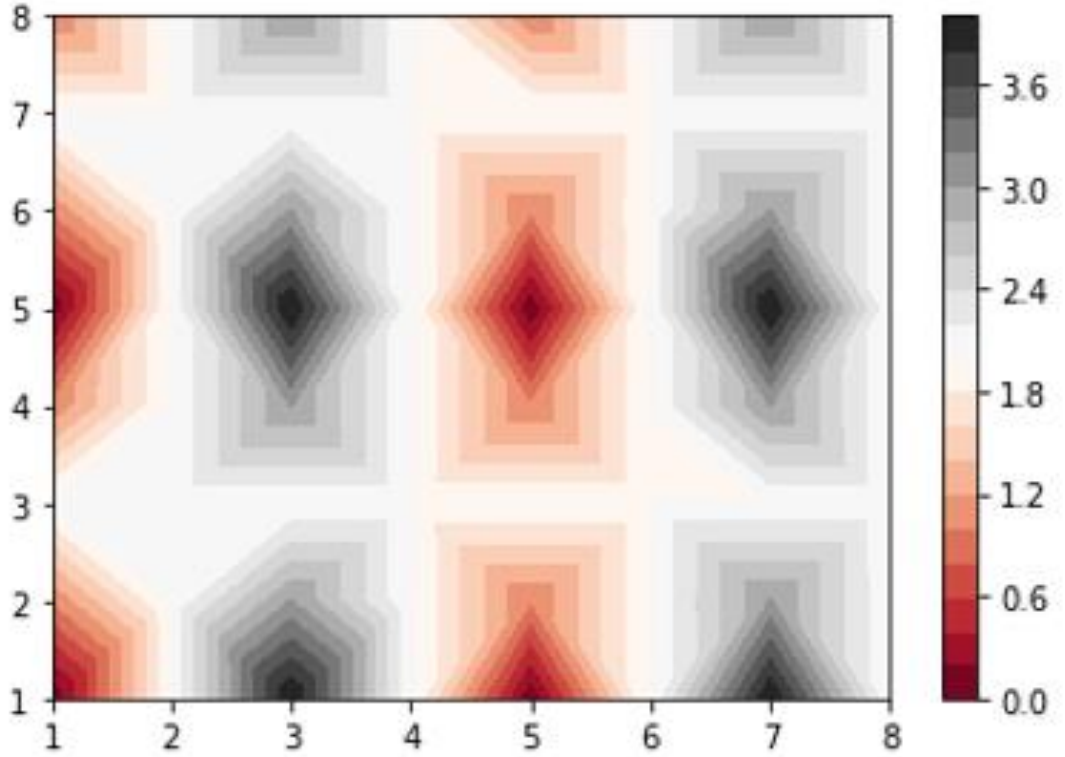


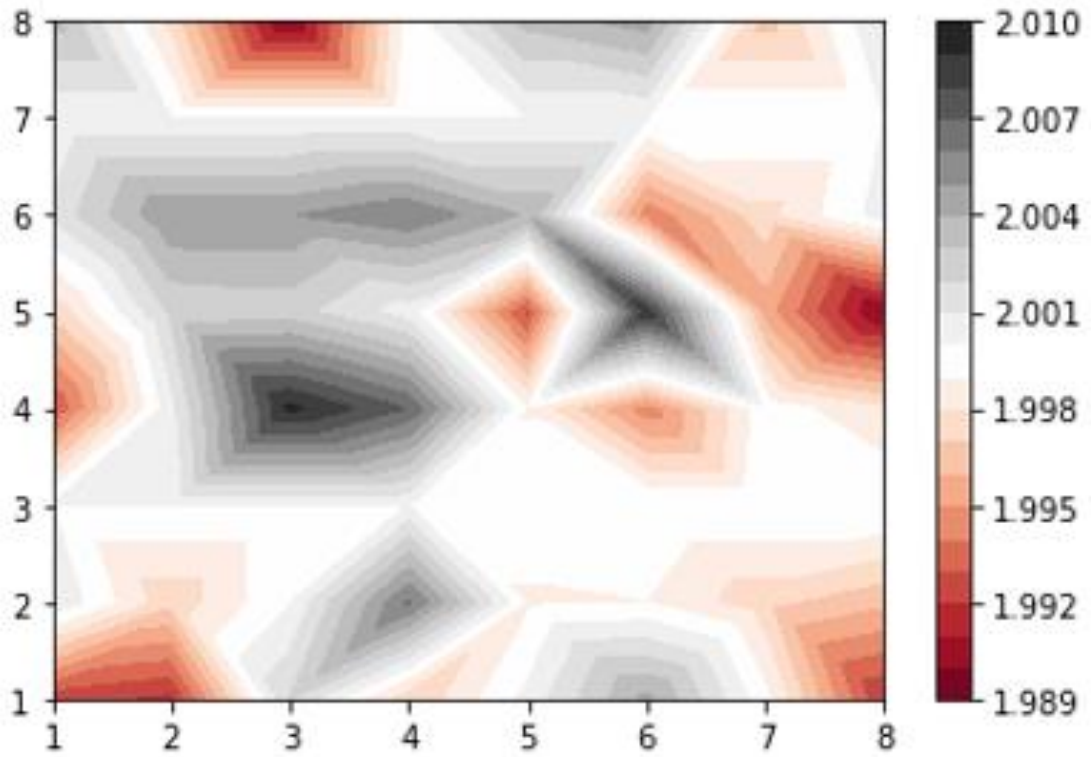


$$E_{II} = \langle\psi_1|I \otimes I|\psi_1\rangle = p_1(|00\rangle) + p_1(|01\rangle) + p_1(|10\rangle) + p_1(|11\rangle) = 1$$

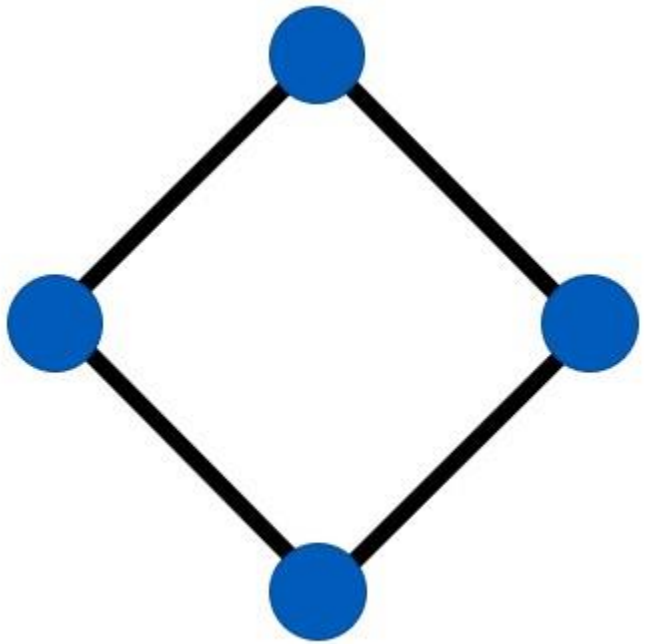
$$E_{IX} = \langle\psi_2|I \otimes Z|\psi_2\rangle = p_2(|00\rangle) - p_2(|01\rangle) + p_2(|10\rangle) - p_2(|11\rangle)$$

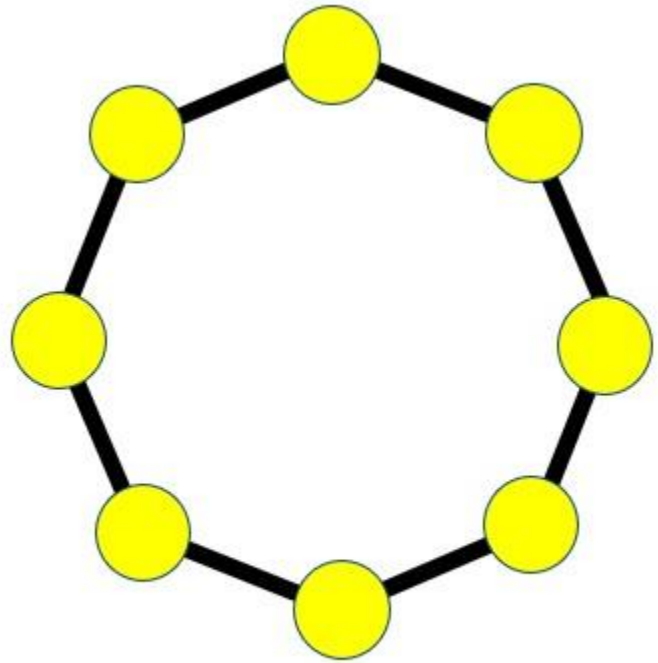
$$E_{XX} = \langle\psi_2|Z \otimes Z|\psi_2\rangle = p_2(|00\rangle) - p_2(|01\rangle) - p_2(|10\rangle) + p_2(|11\rangle)$$

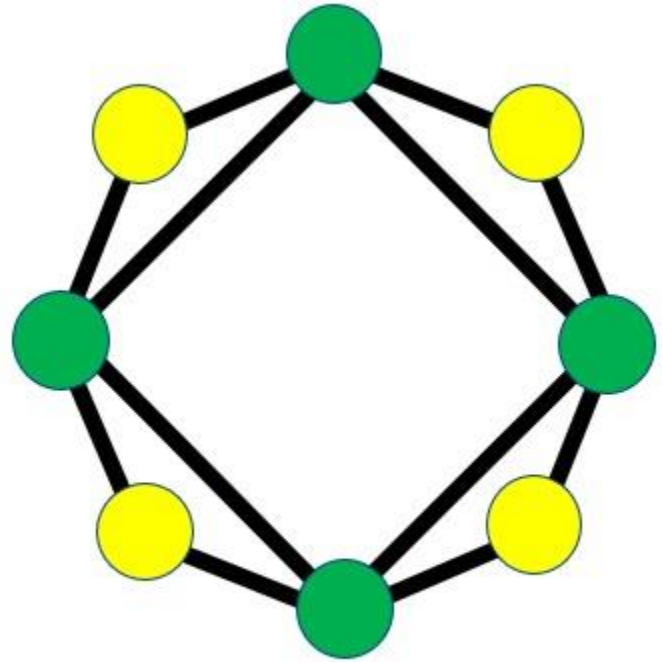


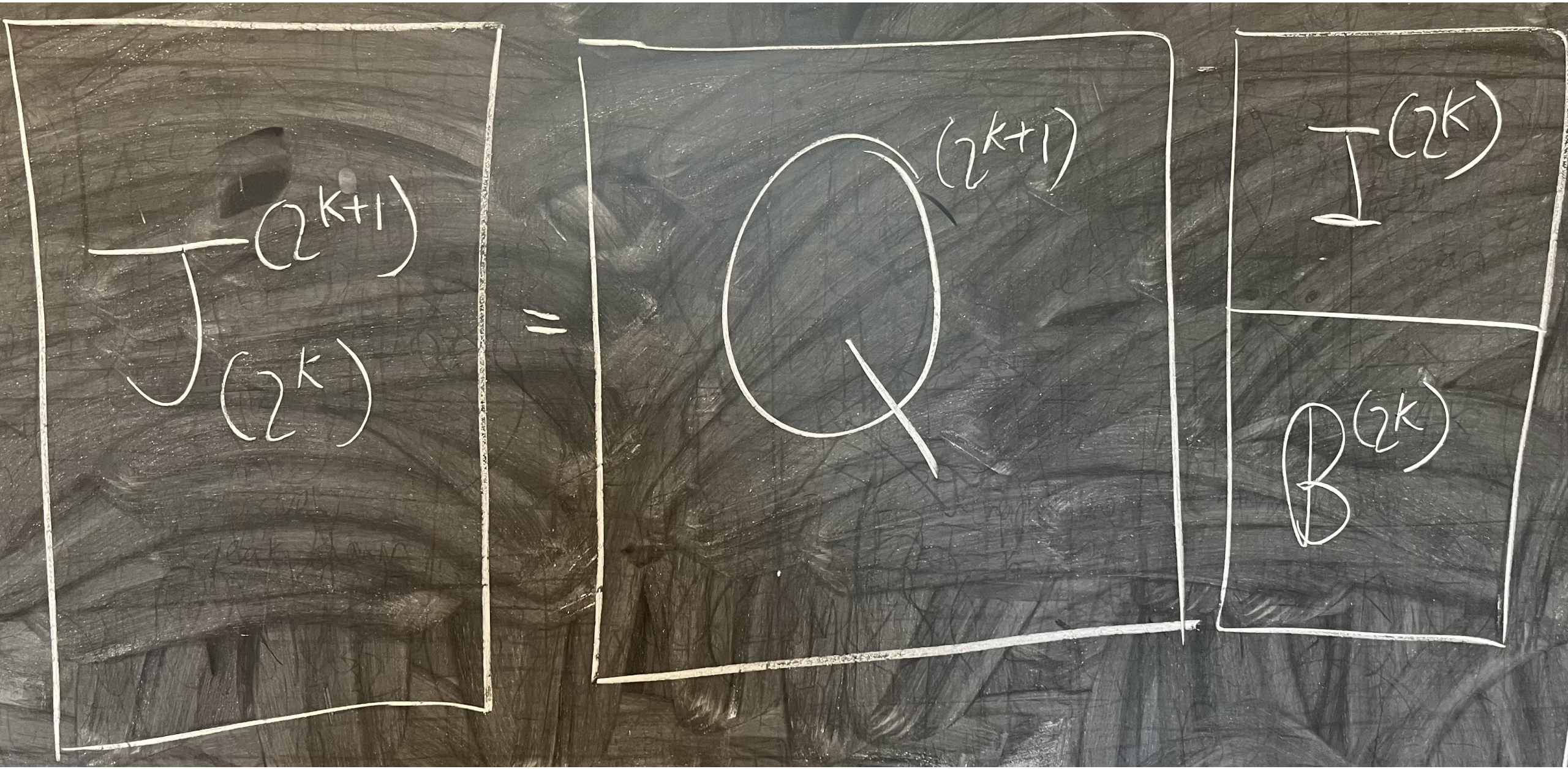


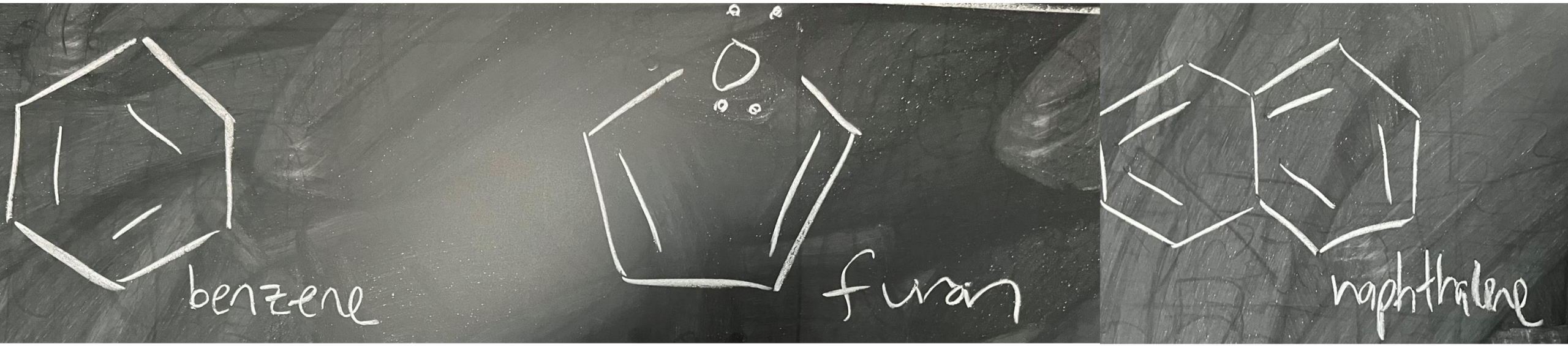
	Eigenvalues	θ_1	θ_2	θ_3
Simulator	0	0	$\pi/2$	$\pi/2$
	4	0	$7\pi/2$	$\pi/2$
	2	$\pi/2$	0	$7\pi/2$
	2	$7\pi/2$	0	$7\pi/2$

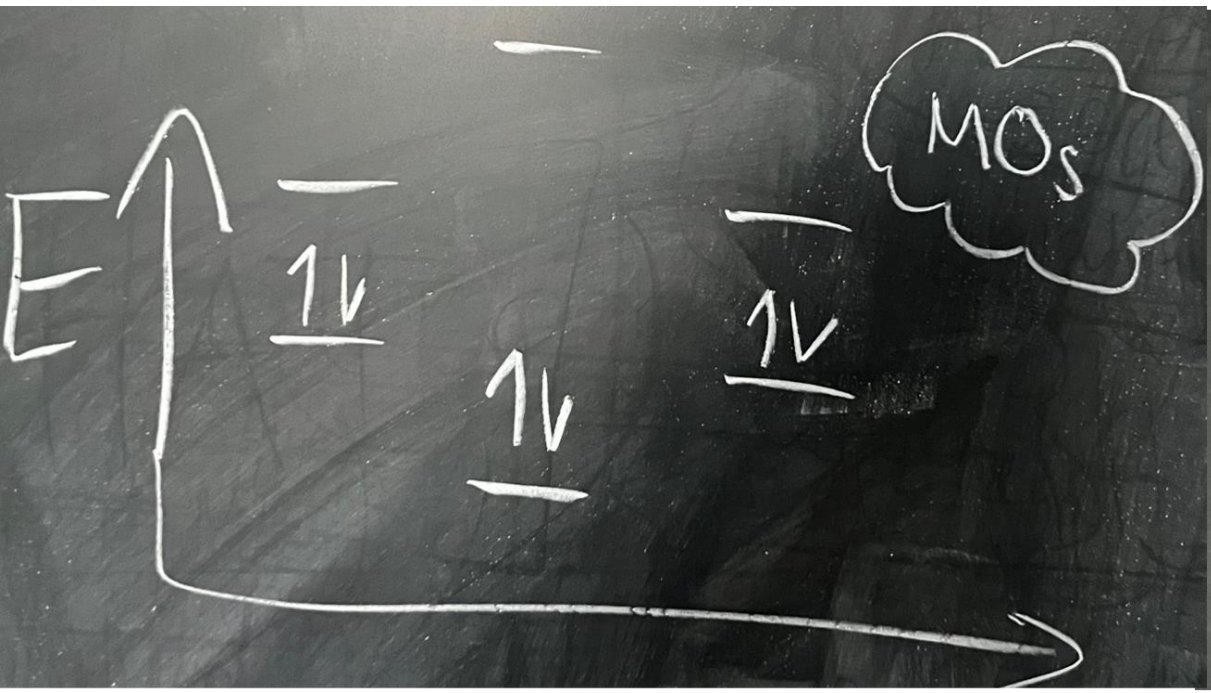


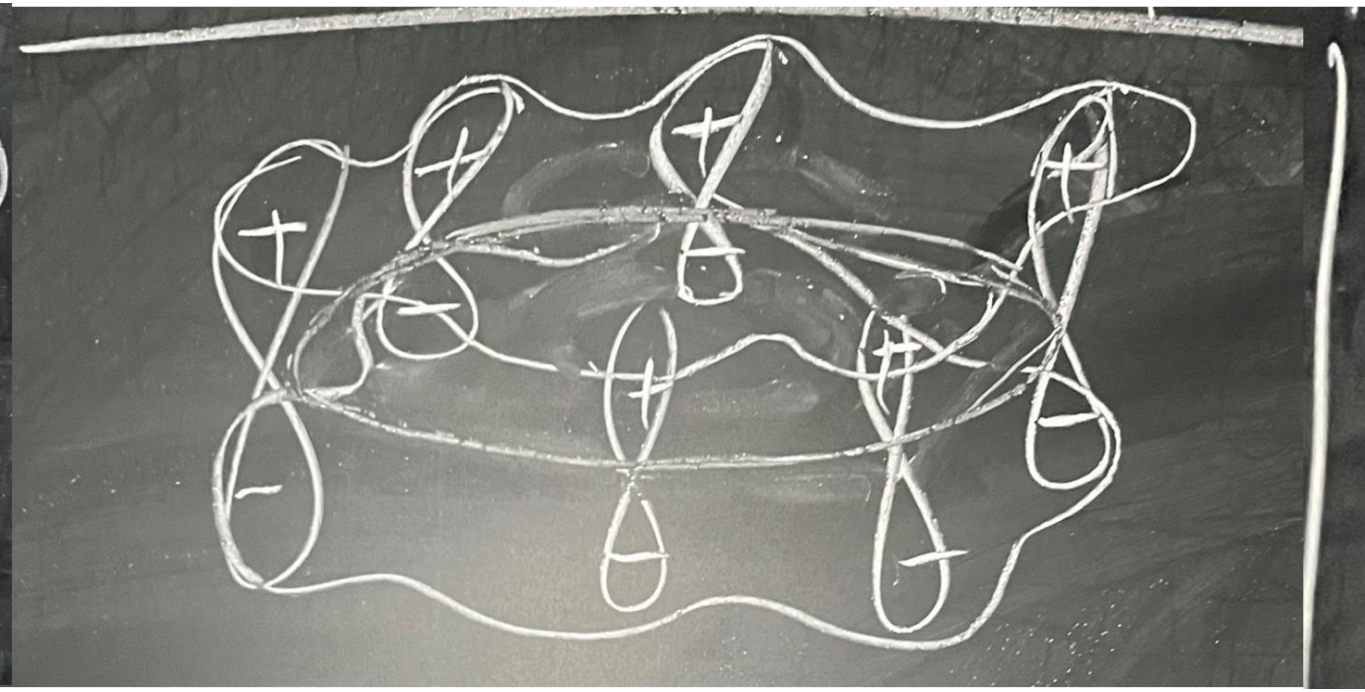




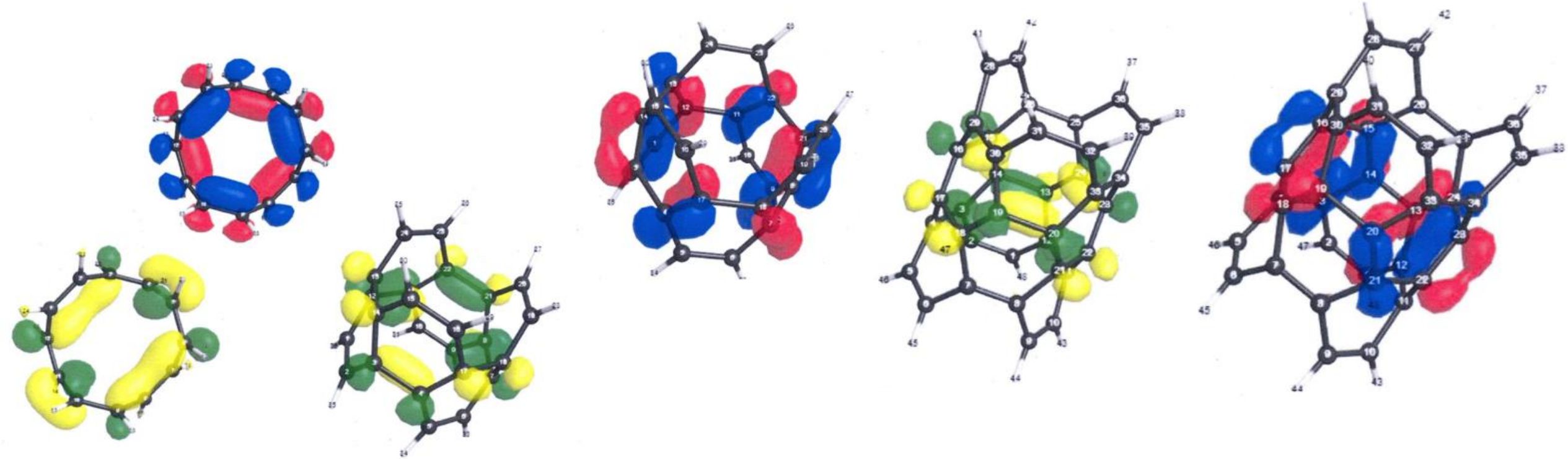

$J^{(2^{K+1})}_{(2^K)}$
=
$Q^{(2^{K+1})}$
$I^{(2K)}$
$B^{(2K)}$

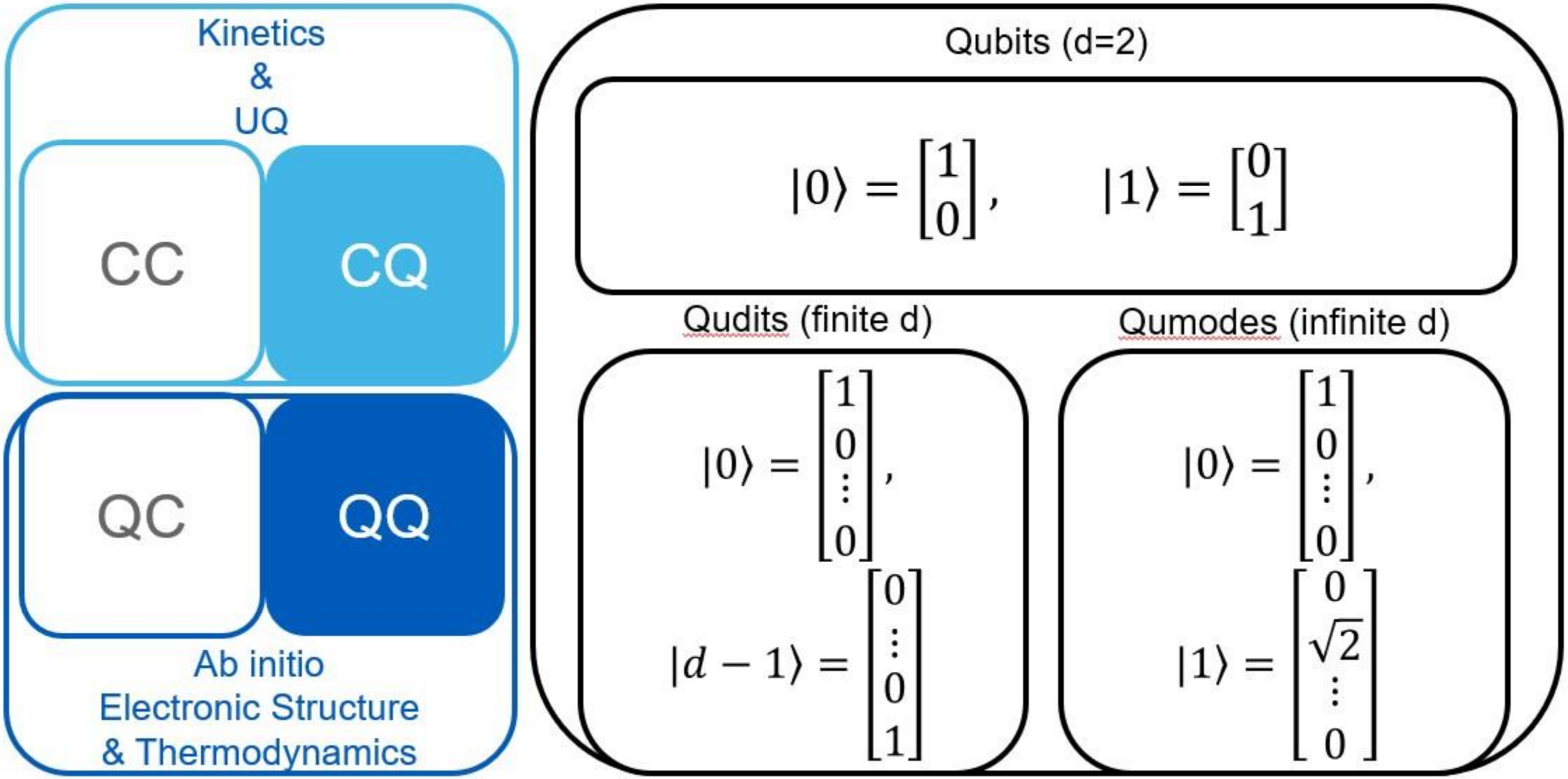

benzene
furan
naphthalene


E
MOs
1↓
1↓
1↓



Made with Avogadro Molecular Editor + Gaussian + WebMO (on UB CCR)




Kinetics
&
UQ
CC
CQ
QC
QQ
Ab initio
Electronic Structure
& Thermodynamics
Qubits (d=2)
$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$
Qudits (finite d)
$|0\rangle = \begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix},$
$|d-1\rangle = \begin{bmatrix}0\\\vdots\\0\\1\end{bmatrix}$
Qumodes (infinite d)
$|0\rangle = \begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix},$
$|1\rangle = \begin{bmatrix}0\\\sqrt{2}\\\vdots\\0\end{bmatrix}$