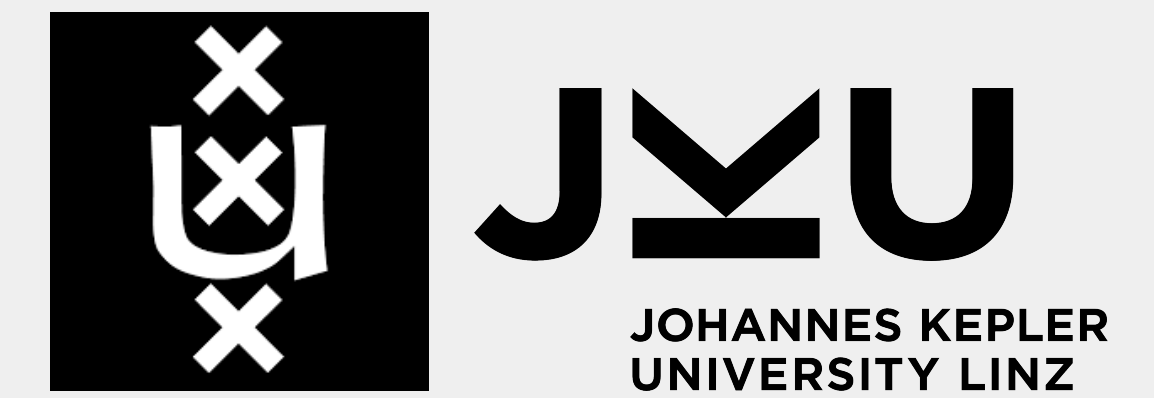


# = Zdb ZigX 7cY F] nhXVaGj Vci ↑ Zh ?b egdkZ ; t3Z; f j kVgVci C ZhV\ Z FVhh^ \

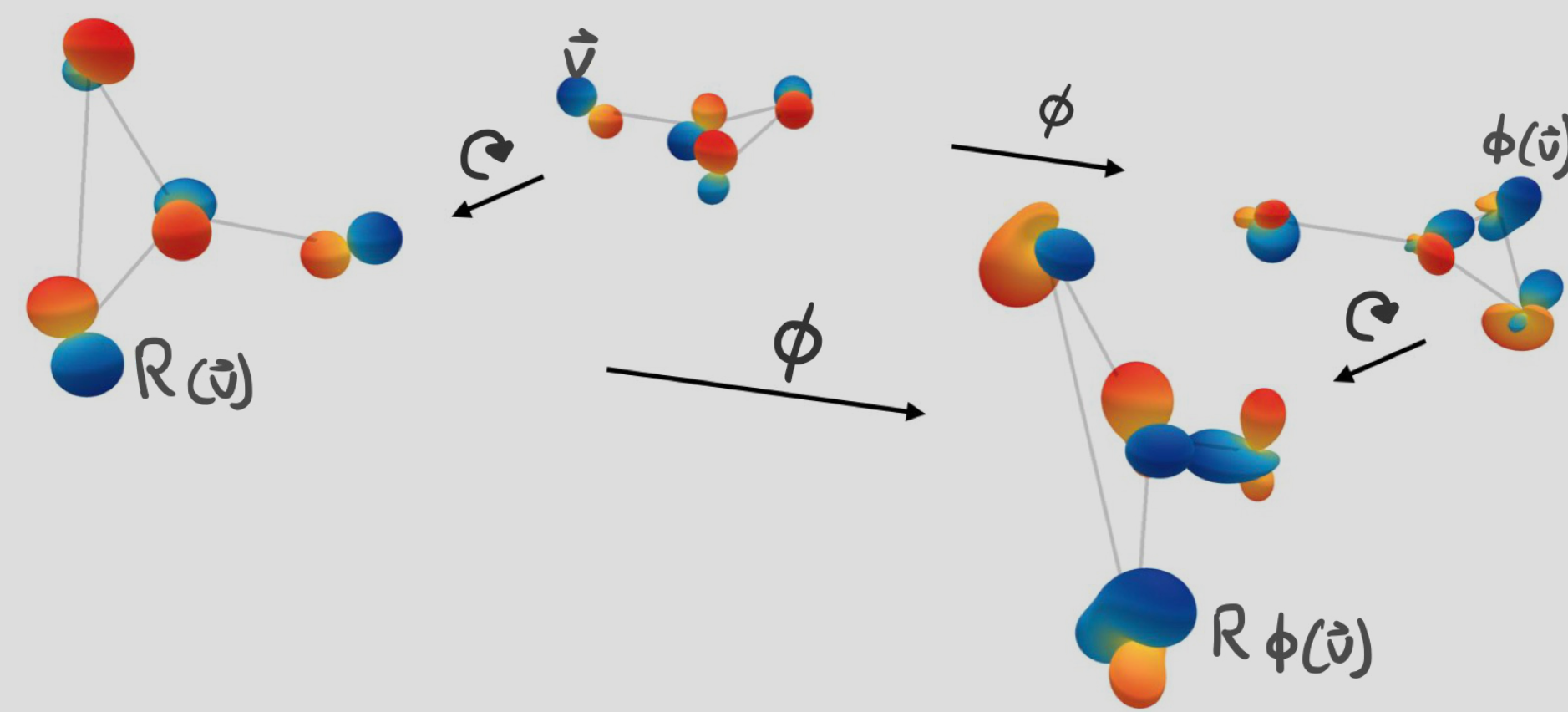
@] VccZh 8gVcYhiZiZg' ( HdW>ZhhZac`z' ; ahZ kVc YZgFdá ; g^ 8Z`Zg^ C VmL Zaæ\`  
 ' J c kZg^tn d[ 7b hiZgVb @] VccZh AZeazgJ c kZg^tn B'co



## KZXidg#Vaj ZY ^[dgp Vi ^dc

9LB", ^ C>YLH†Y>~ L%>L >AY~H>~ s ~>Y'> %BL~BL%o&L" %bα  
 ..., s L} ALH, ^ L>~nL, } L"~B ..pY%>BYL%

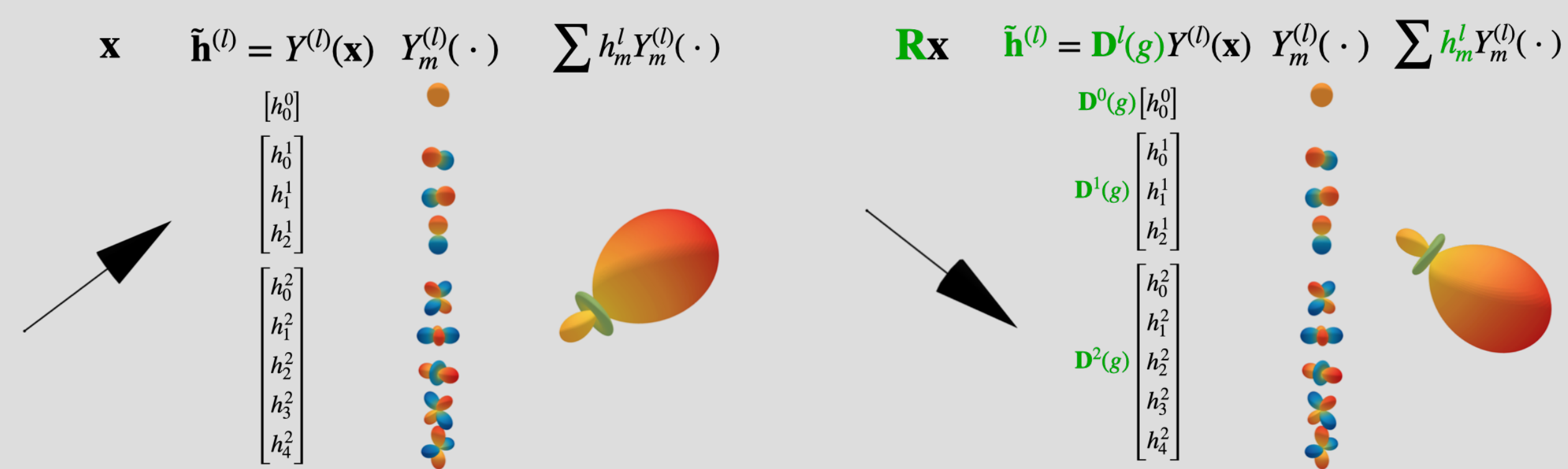
- flαL~H fl 3 L†Y&gt;~s~BL", ε>H%CLB", ^ C>YLH†Y>~ L%oL n N^BL, ^ CL, B'sY
- fl 3 L†Y&gt;~s~BL L†Y&gt;~s~BL ε sp ^L%oLB", ^, ">, ~%o ^>~%o, ~ ^Lj LB, ~%o>~H..L^} Y">, ~%o
- 'Yn} L~"} L%oL >~H~, HL Y..H>L~L"E, ^y%ε sp CLB", ^ C>YLH†Y>~ L%o



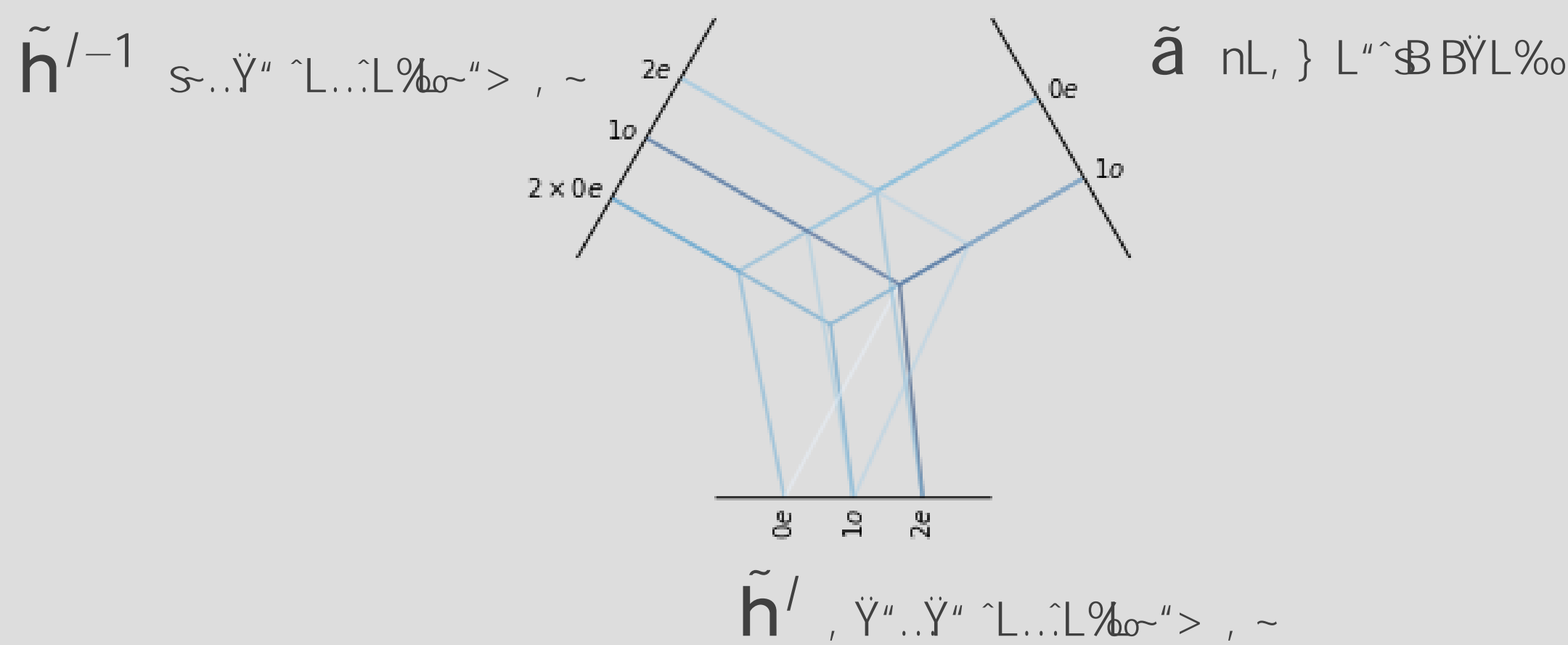
## i ZZg/W&Z [ZVij] gzh" hi ZZg/W&Z kZXidgheVXZh" hi ZZg/W&Z C BFh

&, %o%>ys-n %bL^>AssY ε ^ BL^>s- n^, Y... , AWB" %o^>~%b^ }  
 ε sp } >"^sα CLB", ^ } Y' ..B>, ~

- : L ε, ^y s "pL A>%o%o>~LHA%>qL^B> p>} , ~B%o
- 3.pL^B> p>} , ~B%b} ALHs-n %b†Y&gt;~s~ ε ^ " ^, ">, ~%oε L ε, ^y ε sp %A%o>BL%o ~ ε pBp ^, ">, ~%oB"
- ~ LA%>Z, ^H>~ ~Z "L~%o^ .., HYB" .., C^HL%b†Y&gt;~s~"} >... AL"ε LL~ %bL^>A L CLB", ^ %o>BL%o



## i ZZg/W&Z ; t3Z; f j kVgVci =gVe] DZj gVaDZil dg hti ; =DDhZ



) L%oL m >~H~, HL Y..H>L f ~L"E, ^y%o%o Z "L~%o^ .., H YB" %s~L^L>CLH ε sp ~, ~ s-L>s L%o

$$\tilde{m}_{ij} = \frac{1}{m} \sum_{i,j} \tilde{f}_i \tilde{f}_j \frac{\|x_j - x_i\|^2}{h_{ij}}, \tilde{a}_{ij} = \frac{1}{m} \sum_{i,j} \tilde{f}_i \tilde{f}_j \frac{1}{h_{ij}}; \tilde{f}_i = \frac{1}{m} \sum_{j \in N(i)} \tilde{m}_{ij}, \tilde{a}_i = \frac{1}{m} \sum_{j \in N(i)} \tilde{a}_{ij}$$

## Ddc#a^cZVgkh acZVgXdckdaj i ^dc

	Task Units	α bohr <sup>3</sup>	Δε meV	ε <sub>HOMO</sub> meV	ε <sub>LUMO</sub> meV	μ D	C <sub>v</sub> cal/mol
non-linear	no geometry	NMP	.092	69	43	38	.040
	regular	SchNet *	.235	63	41	34	.033
	steerable	R <sup>3</sup> Cormorant	.085	61	34	38	.038
pseudo-linear	steerable	SE(3) L1Net	.088	68	46	35	.043
	regular	G LieConv	.084	49	30	25	.032
	steerable	SE(3) TFN	.223	58	40	38	.064
pseudo-linear	steerable	SE(3) SE(3)-Tr.	.142	53	35	33	.051
	regular	R <sup>3</sup> × S <sup>2</sup> × R <sup>+</sup> DimeNet++ *	.043	32	24	19	.029
	non-linear	regular	R <sup>3</sup> × S <sup>2</sup> × R <sup>+</sup> SphereNet *	.046	32	23	18
non-linear	regulearable?	SE(3) PaiNN *	.045	45	27	20	.012
non-linear	regular	R <sup>3</sup> EGNN	.071	48	29	25	.029
non-linear	steerable	SE(3) SEGNN (Ours)	.060	42	24	21	.023

Table 2: Comparison on QM9.

- Z^, Y...B, ~C, Y', ~%o ~L ε >Y, ^ "pL, "pL^ LyyL^%o
- ~Y L†Y&gt;~s~" s-L> >Y L^ AL"ε LL~ NL>} >..%o ~ p, } , nL~L, Y%o%o>BL%o%o n^, Y...B, ~C, Y', ~
- 3"LL^>A L C%oL nY' > B, ~C, Y', ~
- "NX G/H yL^~L p>%o%o} L"~Y B, ~%o>s~%o 3Bp\* L" fiZ \*\*
- "HL>, N~, ~ s-L>^ B, ~C, Y', ~ Hs%o%oHs- 3LB, ~
- 2LBL~" ε, ^y A%~ L%o &>~n : LsL^ B } ..LpL~%oL "pL, ^Y >~HB, HL N>} Lε, ^y N^ nL~L^> %bL^>A L ~ \*\* %o

## DZl hiZZg/W&Z VXi kVi ^dc [j cXi ^dch

t^>} s-n } L%oL ..>%oL >%o, ~ s-L>^ B, ~C, Y', ~>, ε %Y%o, %oL  
 "pL ~, HL Y..H>L >%oLε L†Y&gt;~s~" >B C>, ~ N^B, ~

$$\tilde{f}_i = \frac{1}{m} \sum_{j \in N(i)} \tilde{m}_{ij} \tilde{a}_j$$

' B C>, ~ N^B, ~>%o, ~ s-L>^ ) &/%ε pBp >L >...ε H~, HL ε %o

## FZgdg VcXZ VcY VeaXVWa^tn

3fiZ \* \* %ε, ^y L%oL B> Y ε L ε pL~ "pL^L %o.pY%>B> >~H nL, } L"~B>  
 s-N^ } >, ~ >C>s>A L

- fl~Bp %bL^ ~, HL Y..H>L%>C L, B'sY N^BL } , } L~"Y' >BBL L^>, ~ %o> >~nY' >} , } L~"Y'
- fl~Bp %bL^ } L%oL %>L > CL .., %o, ~ L > CL N^BL%>Hs.. L } , } L~" %o

) L"p, H ) 3fi

3fi 5^

5t \*

\* ) /

2>Hs t ε H

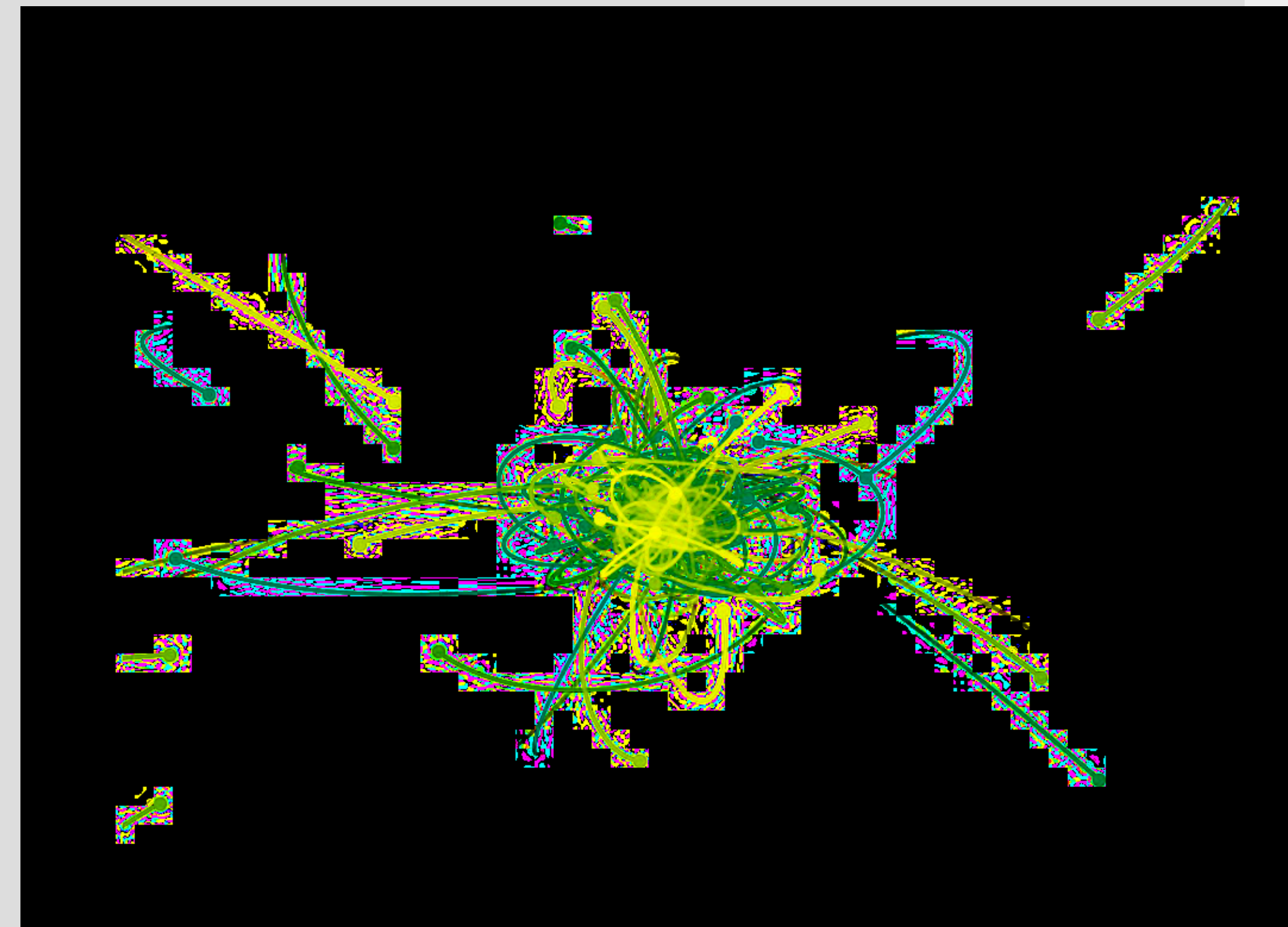
fiZ \*\*

3fi s-L>

3fi ~ s-L>

3fiZ \*\* z

3fiZ \*\* z /



## HZ[Zg^cXZh

fl'sy \$, LyyL~%o  
 . %oL B~%o ~ ε n^, Y..%o  
 " ~L^>, ~>, ~NL~BL, ~εL>~s-n 2L..L%o>, ~%o  
 ) >s ZLsL^ εL%o} &+ ^ AY) (L~W) s~Y^\*) sL^: ^Y^L^, ) %o>, ^HLy/ εL %o>~Y- &~.BpL%o%o) >Y^εL: LsL^ ) Bp<  
 5%yε ε ε B; 3; , ~>L~L %oL %o~ \* Y'ssY~n 3, ..ps 3>~A, ~ \$ %o 2>BYL^%o~H) Bp>L, >LY  
 L ~L ~