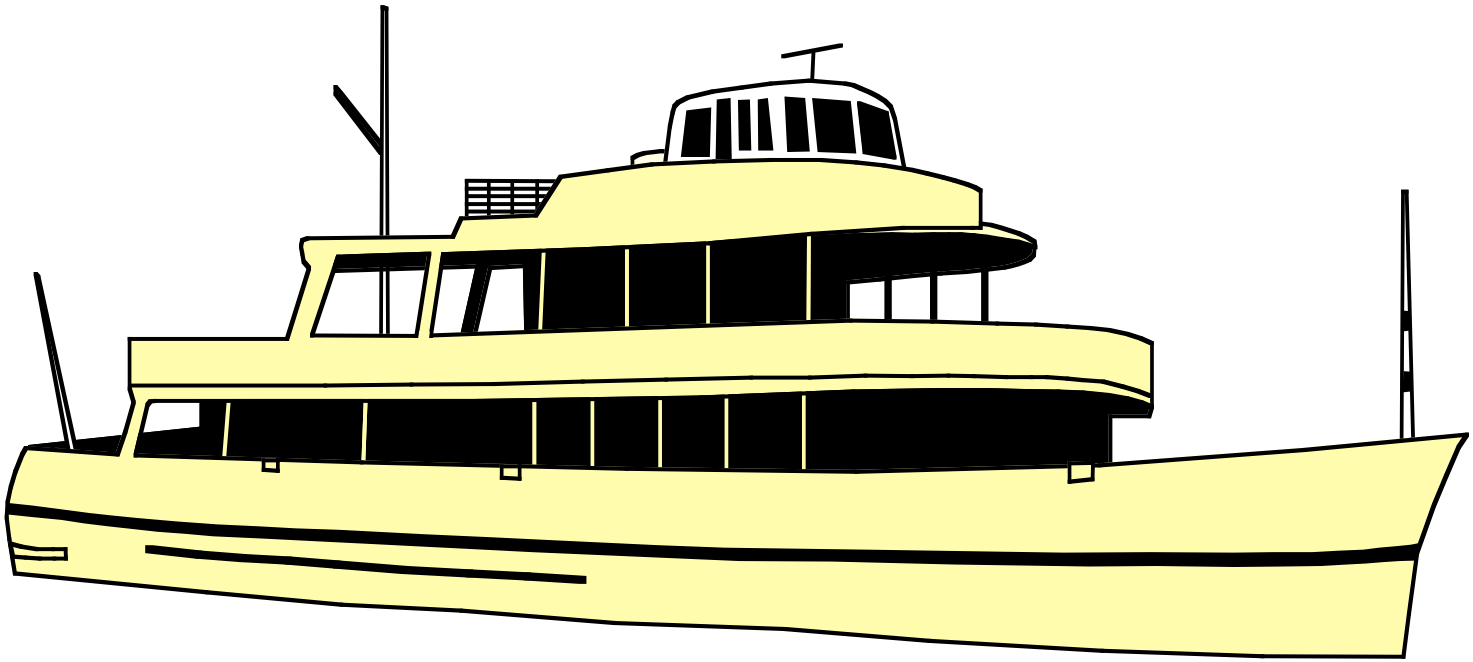
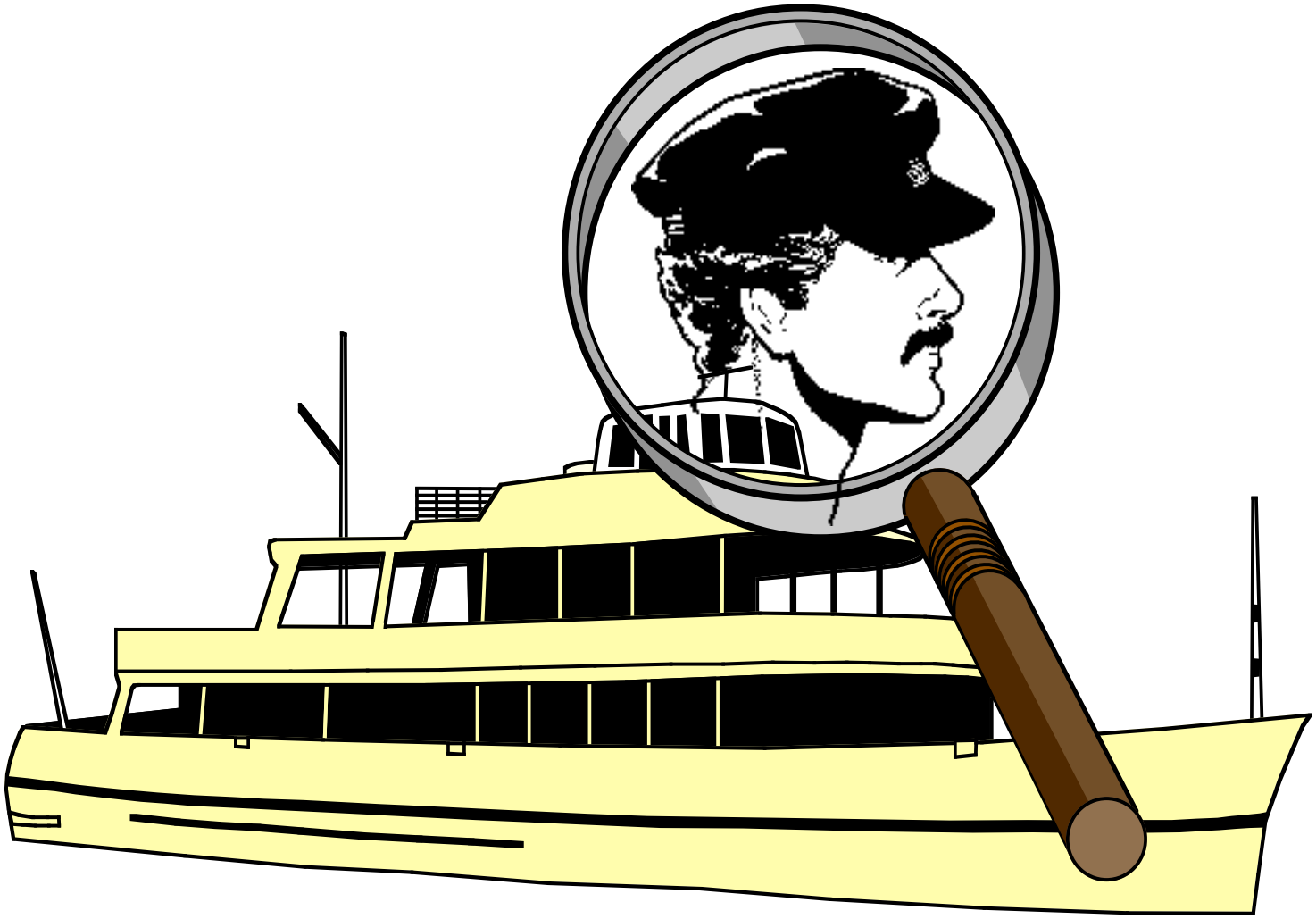
VB-ICF
Is there BSSE in VB



Measure weight of ship

He_2-ICF



1 Hartree = 627.5 Kcal/mol

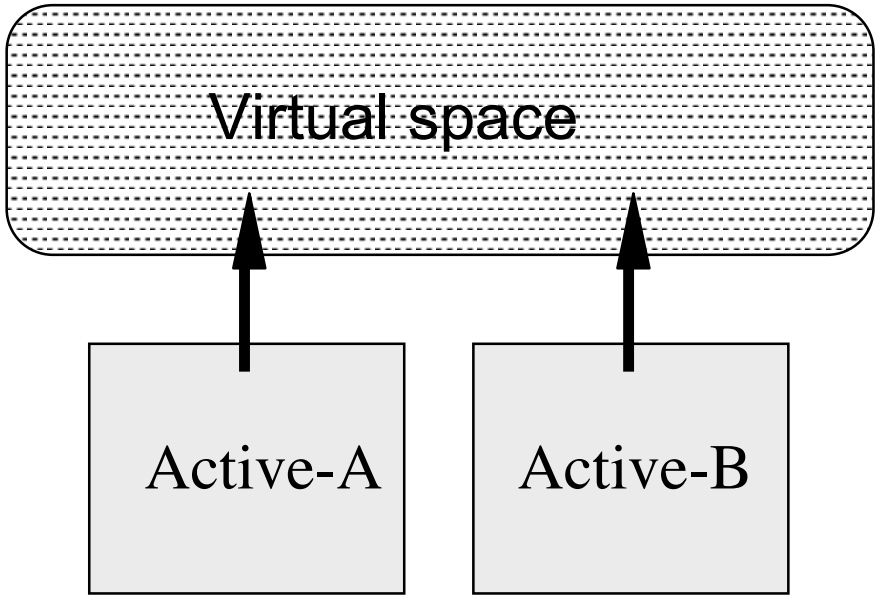
Determine weight of captain by weighing ship - captain

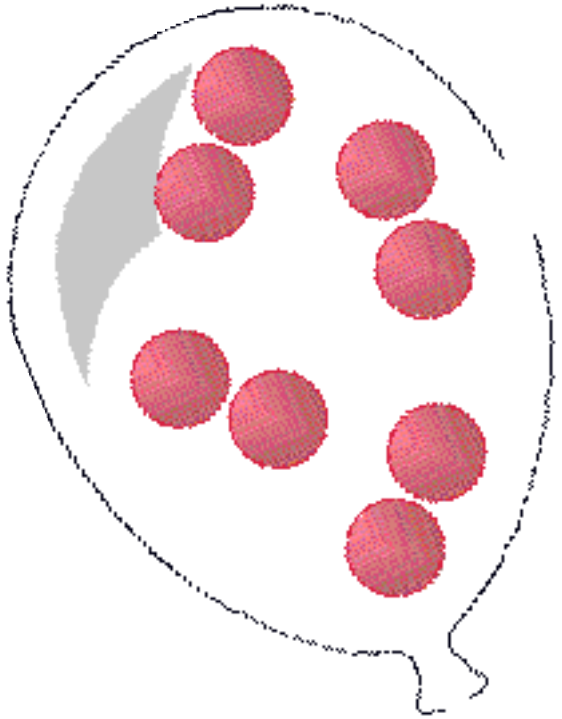
1 Hartree = 315777 Kelvin

Determine the weight of the star on his cap using the same procedure

He_2

Interacting Correllated Fragments (Liu/Mclean)





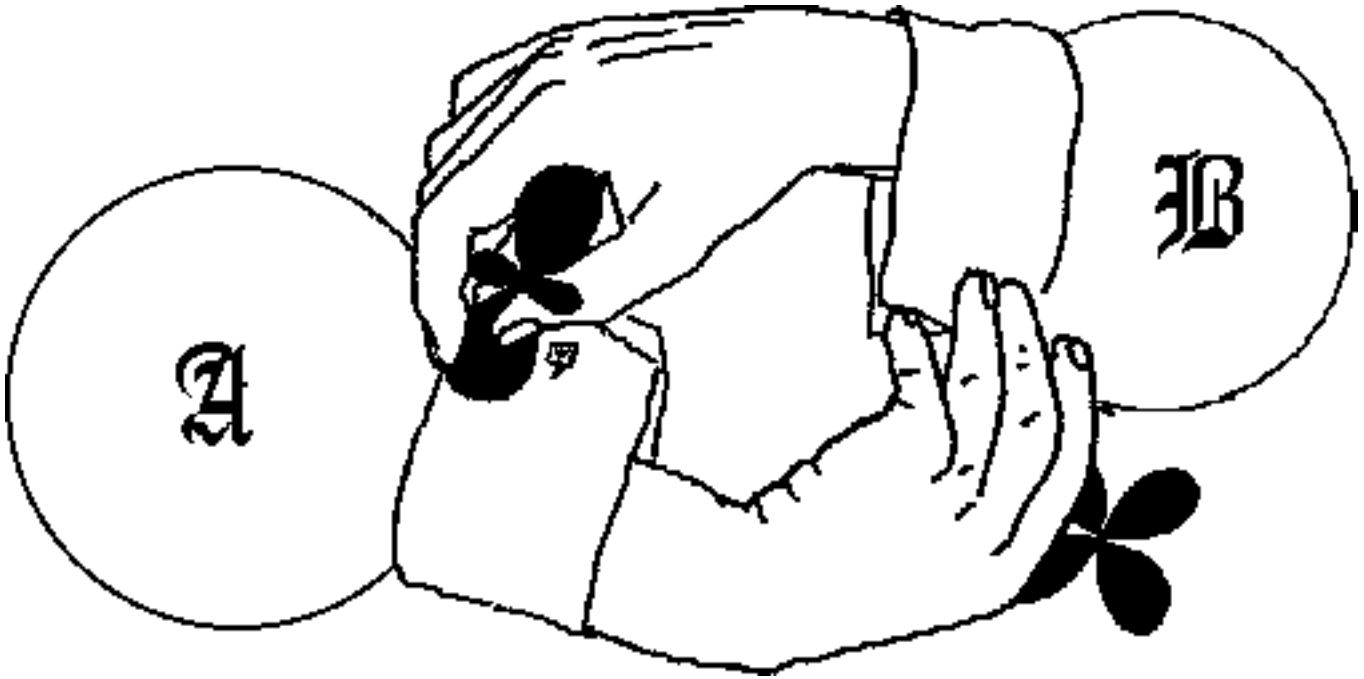
ICF1 : 1s

ICF2 : 1s,2sp

ICF3 : 1s,2sp,3spd

BASIS SET

C1D2 - (15 → 6)s2p1d/1p1d (50 AO's)



F,B. van Duineveldt, naar "Tekenen" ,M.C. Escher (1948)

Helium dimer (MRCI) (K)

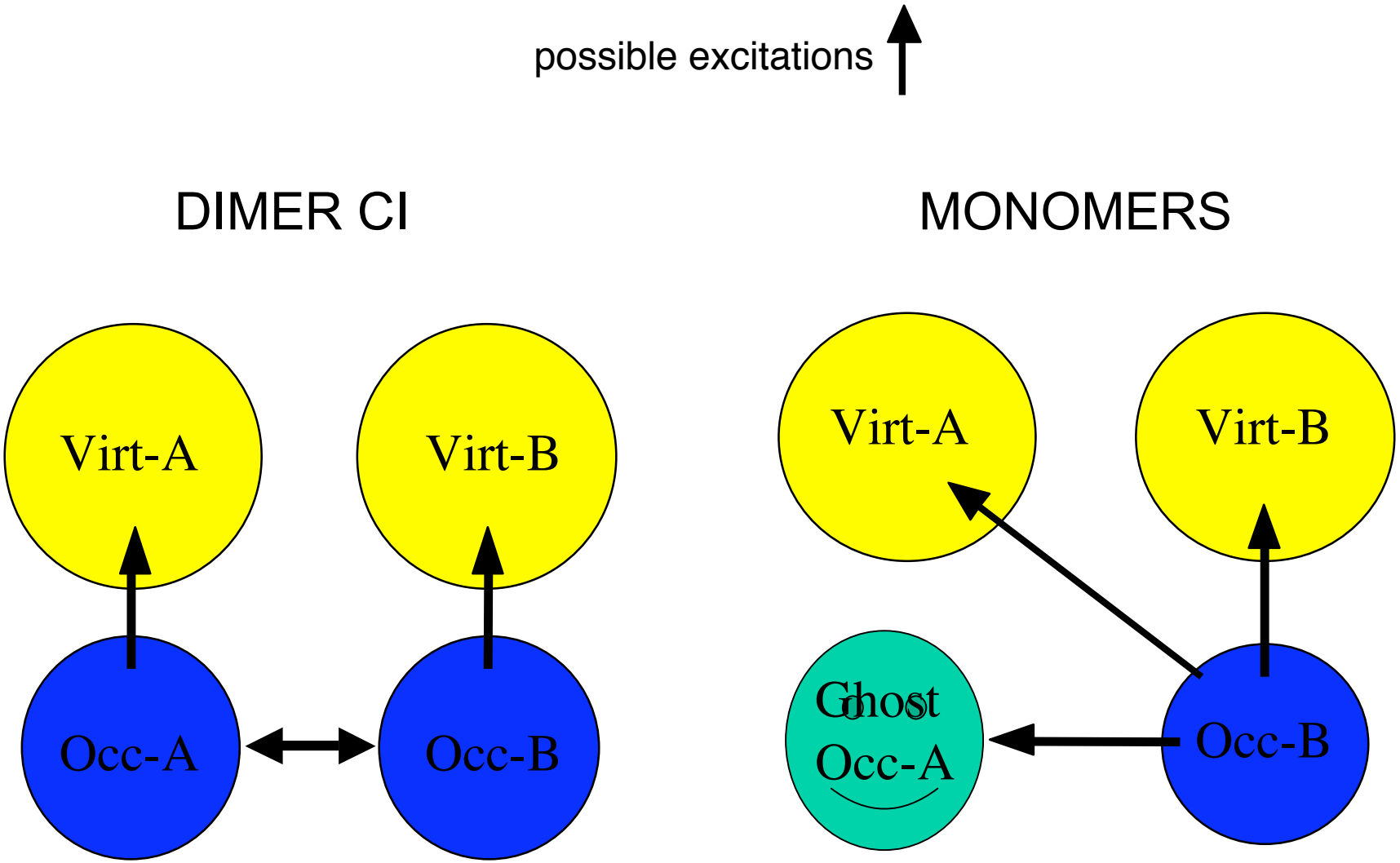
	5.6 bohr		4.0 bohr	
	C1D2	C3D5BF	C1D2	C3D5BF
E_{int}	-9.08	-10.86	323.1	296.3
BSSE	2.09	12.56	5.7	23.3

VB may be
restricted
to be strictly local
but .....

Counterpoise

S.F. Boys, F. Bernardi Mol. Phys. 19 (1970) 553

possible excitations



Interaction energies for He_2 (in K) at 5.6 Bohr using C1D2 .

Model	ΔE	ΔE (just Orbital-corrected)
fulll CI	-9.08	-10.13*
MO-ICF1	-9.73	-11.16
MO-ICF2 (**)	-9.07 (-9.88)	
VB-ICF1 (local dispersion)	-8.60	-10.02
VB-ICF1	-10.75	-12.17
VB-ICF2	-9.75	-9.91

* This is the uncorrected full CI result; The difference between Orbital and the rest is not clear at the full CI level

** Best shot (other shot); Vos et al , Mol. Phys.,67,1011 (1989)

Atomic correlation energy (monomer) ≈ 0.04 Hartree ≈ -12585 K