

from toy model to quantum physics

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1

Overview for the charge-charge case

order	multipole moment / field	first order quasi moment / quasi field	second order quasi moment / quasi field	...
$\mathcal{O}(0)$	$M \propto r^0 Y_{00}$ $V \propto r(0)$ } MI [a]	$M^{(1)} \propto \{r^1 Y_{00}\}$ $V^{(1)} \propto \Delta r(0)$ } MS ⁽¹⁾ [d]	$M^{(2)} \propto \{r^2 Y_{00}\}$ $V^{(2)} \propto \Delta^2 r(0)$ } MS ⁽²⁾
$\mathcal{O}(2)$	$Q \propto r^2 Y_{20}$ $V_{ij} \propto \partial_{ij} r(0)$ } QI [b]	$Q^{(1)} \propto \{r^2 Y_{20}\}$ $V_{ij}^{(1)} \propto \partial_{ij} \Delta r(0)$ } QS ⁽¹⁾ [e]	$Q^{(2)} \propto \{r^3 Y_{20}\}$ $V_{ij}^{(2)} \propto \partial_{ij} \Delta^2 r(0)$ } QS ⁽²⁾
$\mathcal{O}(4)$	$H \propto r^4 Y_{40}$ $V_{ijkl} \propto \partial_{ijkl} r(0)$ } HDI [c]	$H^{(1)} \propto \{r^4 Y_{40}\}$ $V_{ijkl}^{(1)} \propto \partial_{ijkl} \Delta r(0)$ } HDS ⁽¹⁾	$H^{(2)} \propto \{r^5 Y_{40}\}$ $V_{ijkl}^{(2)} \propto \partial_{ijkl} \Delta^2 r(0)$ } HDS ⁽²⁾
...

Corrections due to the shape of the nucleus (quadrupole moment) in the case without overlap

2

Exactly solvable classical toy model : no electrons in nucleus

Interaction Energy ($e^2/4\pi\epsilon_0$)

$E_0(\theta) = -2C \left(\frac{1}{\sqrt{\ell^2 \sin^2 \theta + (d - \ell \cos \theta)^2}} + \frac{1}{\sqrt{\ell^2 \sin^2 \theta + (d + \ell \cos \theta)^2}} \right)$ $C = e^2 / (4\pi\epsilon_0)$

3

$E(\theta) = 2 \left(\frac{-e^2}{4\pi\epsilon_0} \right) \left(\frac{1}{r_a} + \frac{1}{r_b} \right)$

$= 2 \left(\frac{-e^2}{4\pi\epsilon_0} \right) \left(\frac{1}{\sqrt{\ell^2 \sin^2 \theta + (d - \ell \cos \theta)^2}} + \frac{1}{\sqrt{\ell^2 \sin^2 \theta + (d + \ell \cos \theta)^2}} \right)$

4

	$l=0$	$l=1$	$l=2$
nucleus	charge	dipole moment	quadrupole moment
electrons	electric potential	electric field	electric-field gradient (EFG)
	(scalar)	(vector)	(rank 2 tensor)

5

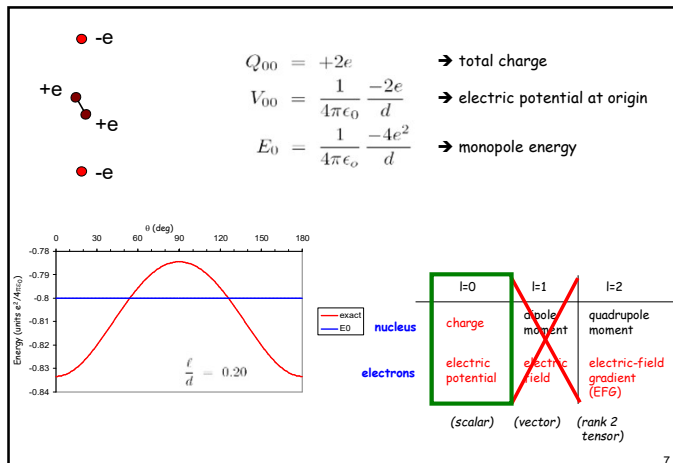
$Q_{00} = +2e \rightarrow$ total charge

$V_{00} = \frac{1}{4\pi\epsilon_0} \frac{-2e}{d} \rightarrow$ electric potential at origin

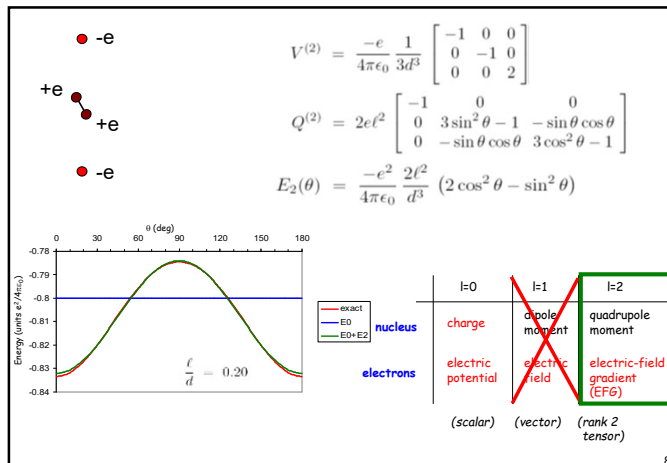
$E_0 = \frac{1}{4\pi\epsilon_0} \frac{-4e^2}{d} \rightarrow$ monopole energy

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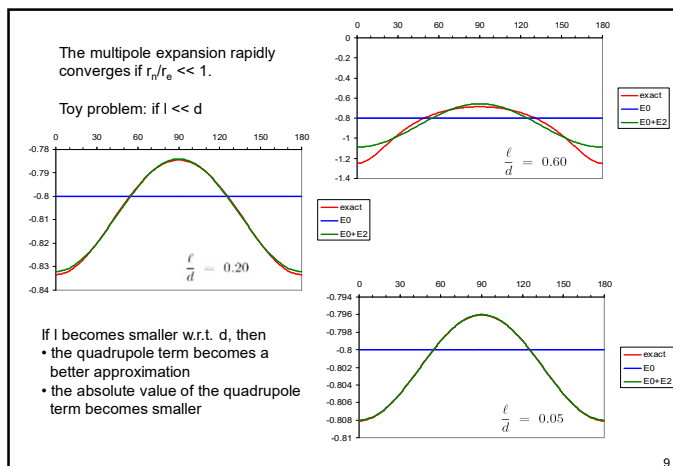
6



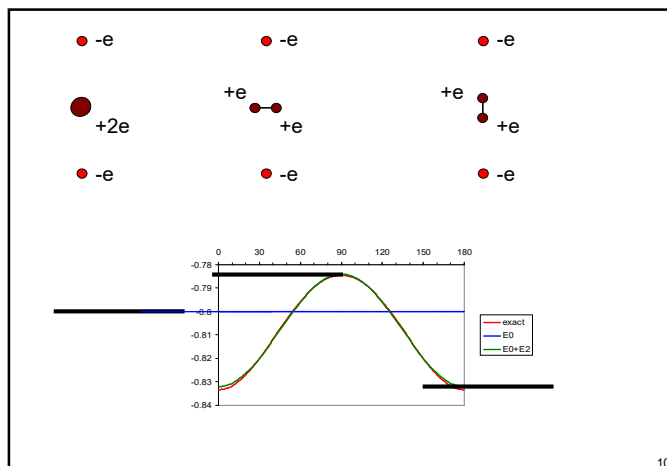
7



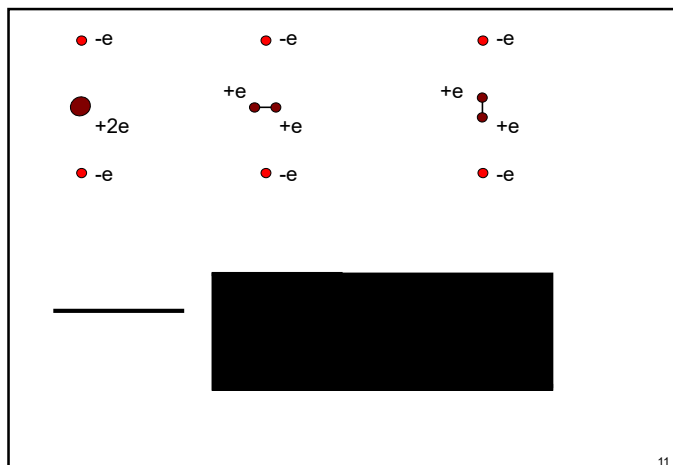
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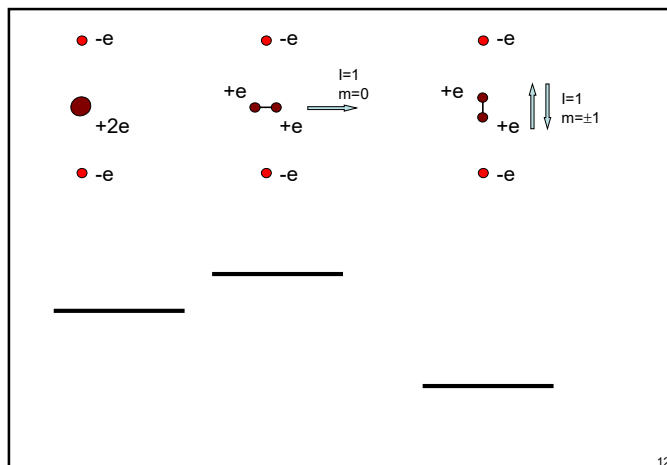
9



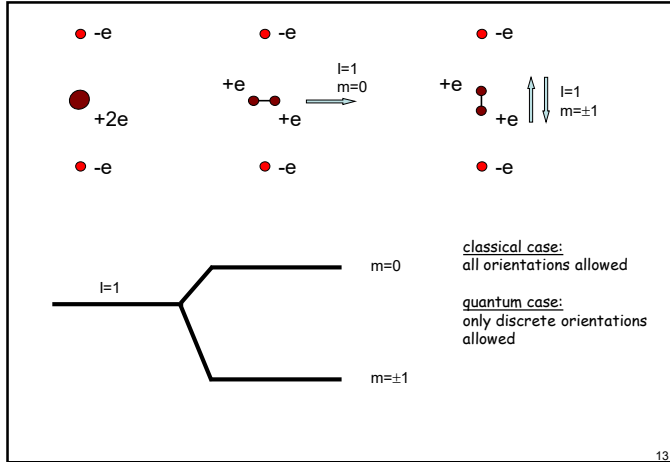
10



11



12



13