Physics 243A—Surface Physics-
Spectroscopy
Suggested answers to Problem Assignment 2

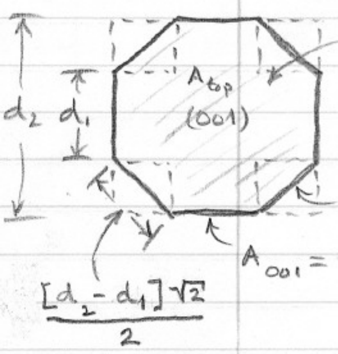
All of PS 2, plus 3.1 and 3.2

[2.1] TWO CONDITIONS MUST BE SATISFIED:

(a) ① MINIMIZE TOTAL FREE ENERGY $= \int \gamma \, dA = \underbrace{\sum_i \gamma_i A_i}_{\text{ALL FACES}}$
WITH t = CONSTANT

② DURING MINIMIZATION HOLD NO. ATOMS $\equiv N = \rho V$ = CONSTANT

WRITING THESE OUT IN MORE DETAIL FROM GEOMETRY OF ISLAND:



$A_{top} = d_2^2 - 2\left\{\frac{[d_2-d_1]}{2}\right\}^2$

$A_{011} = 4\frac{[d_2-d_1]}{\sqrt{2}} \cdot t = 2\sqrt{2}[d_2-d_1]t$

$A_{001} = 4 d_1 \cdot t$

$$\therefore \; G = \gamma_{001} A_{top} + \gamma_{001} A_{001} + \gamma_{011} A_{011} + \overset{0}{\cancel{\gamma_{ISLAND-SUBSTRATE}}} A_{top}$$

$$= \gamma_{001}\left[d_2^2 - 2\left\{\frac{[d_2-d_1]}{2}\right\}^2 + 4 d_1 t\right] + \gamma_{011} 4\frac{[d_2-d_1]}{\sqrt{2}} t \qquad ①$$

$$V = A_{top} t = \left[d_2^2 - 2\left\{\frac{[d_2-d_1]}{2}\right\}^2\right] t$$

$$= \text{CONSTANT} \qquad ②$$

BUT, WITH t = CONSTANT $\equiv t_0$

$$A_{top} = \text{CONSTANT}$$

$$\equiv A_0$$

$$= d_2^2 - 2\left\{\frac{[d_2-d_1]}{2}\right\}^2 \qquad ③$$

WHICH ALSO RELATES d_1 AND d_2

THUS, $$G = \underbrace{\gamma_{001}[A_0}_{} + 4 d_1 t_0] + \gamma_{011} 4\frac{[d_2-d_1]}{\sqrt{2}} t_0$$

$$= G_0 + 4\left[\gamma_{001} t_0 d_1 + \frac{\gamma_{011}}{\sqrt{2}} t_0 [d_2-d_1]\right] \equiv G_0 + \Delta G$$

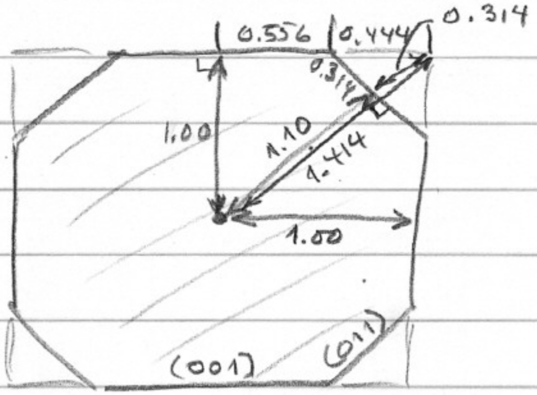
SO JUST NEED TO MINIMIZE

$$\Delta G = \gamma_{001} d_1 + \frac{\gamma_{011}}{\sqrt{2}}[d_2-d_1] = d_1\left[\gamma_{001} + \frac{\gamma_{011}}{\sqrt{2}}\left[\frac{d_2}{d_1} - 1\right]\right]$$

$$= d_1\left[1.00 + 0{,}778\left[\frac{d_2}{d_1} - 1\right]\right]$$

WITH d_1 AND d_2 RELATED VIA ③, A QUADRATIC EQUATION, SO AS TO YIELD SINGLE VARIABLE d_1.

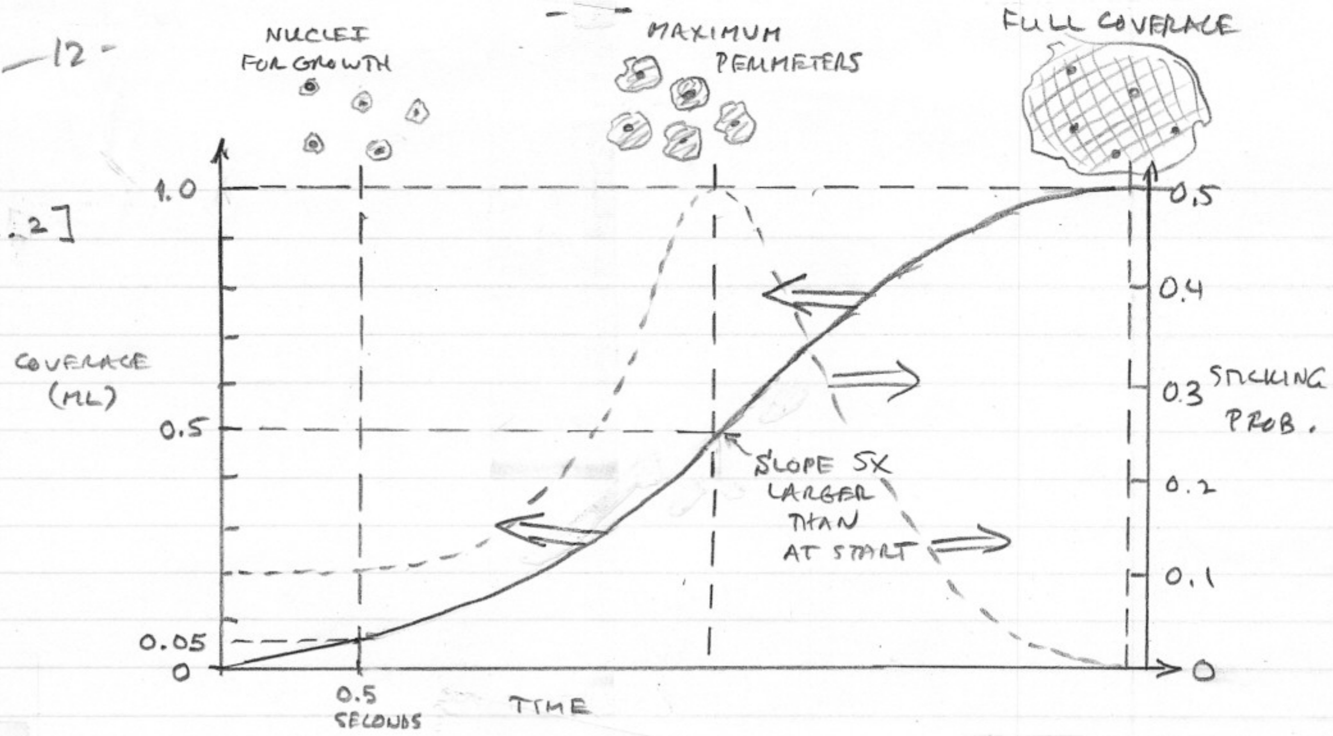
[2.1] (b) WULFF CONSTRUCTION FOR THIS TWO-SURFACE → "TWO-EDGE" SURFACE LOOKS LIKE:



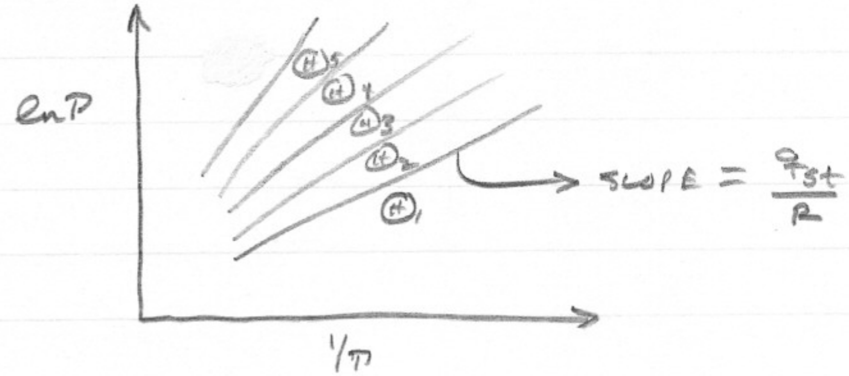
WHERE WE HAVE SOLVED THE TRIANGLE IN UPPER RIGHT TO DERIVE THE NOS. SHOWN. ∴ RATIO $\frac{A_{011}}{A_{001}} = \frac{0.314}{0.556} = \underline{\underline{0{,}564}}$

↓

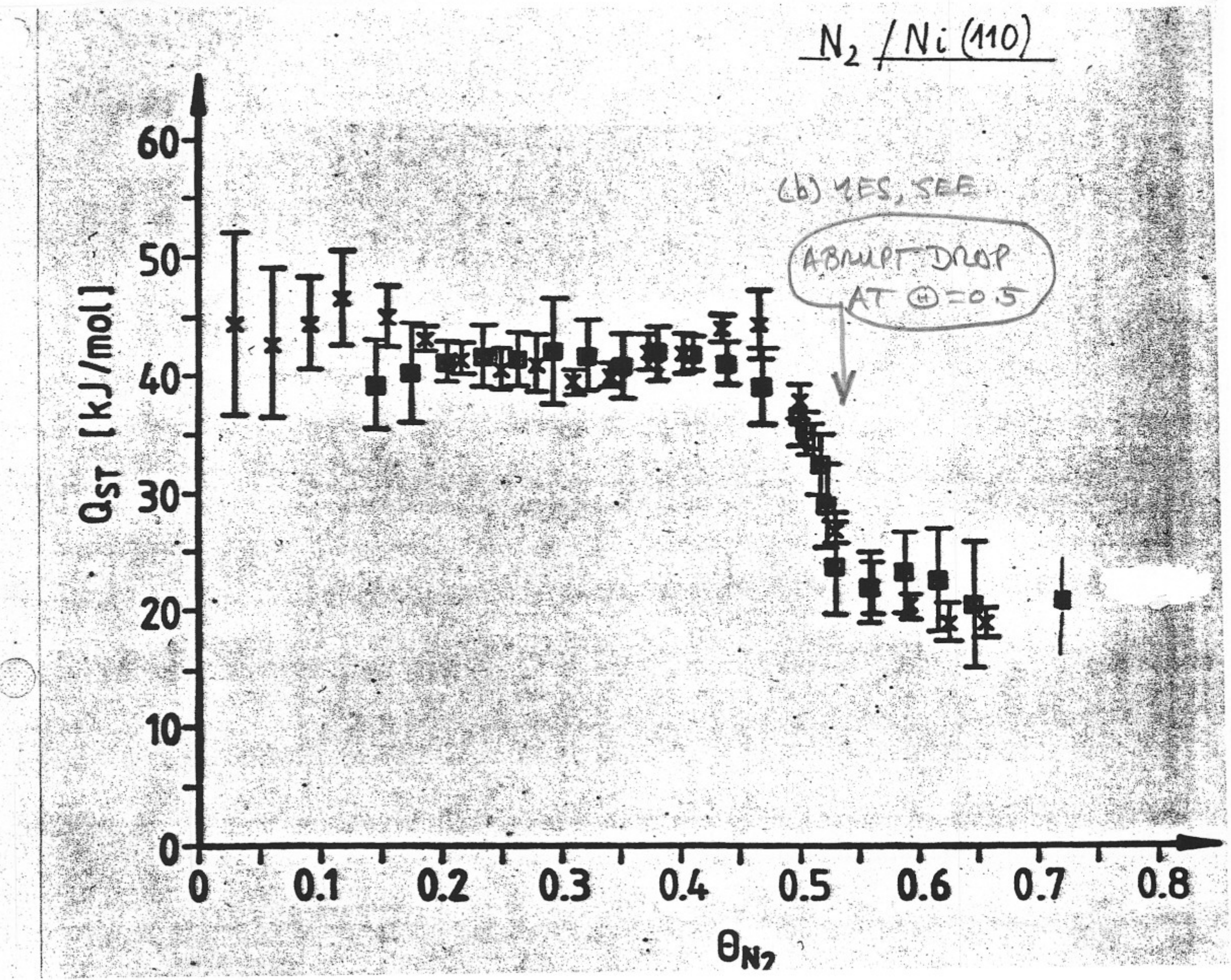
[2.2]


NUCLEI FOR GROWTH
MAXIMUM PERIMETERS
FULL COVERAGE
1.0
0.5
0.05
0
COVERAGE (ML)
0.5 SECONDS
TIME
0.5
0.4
0.3
0.2
0.1
0
STICKING PROB.
SLOPE 5X LARGER THAN AT START

[2.3] (a) CHOOSE FOR A GIVEN N1s = Θ VALUE (P, T) PAIRS AND THEN PLOT DATA AS:



FINALLY GIVES CURVE AS BELOW



(b) YES, SEE ABRUPT DROP AT Θ = 0.5

[2.4] THE LANGMUIR ISOTHERM LOOKS LIKE:

$$\frac{\Theta}{\Theta_{SATN}} = \frac{P}{\left(\frac{k_2}{k_1}\right) + P} = \frac{P}{P_{1/2}(T) + P}$$

(LECTURE) (ZANGWILL EQ. 9.6)

OR LINEARIZED AS:

$$\frac{\Theta_{SATN}}{\Theta} = \frac{\left(\frac{k_2}{k_1}\right) + P}{P} = 1 + \left(\frac{k_2}{k_1}\right) P^{-1} \; ; \; \frac{1}{\Theta} = \frac{1}{\Theta_{SATN}}\left[1 + \left(\frac{k_2}{k_1}\right) P^{-1}\right]$$

CHECK FOR APPLICABILITY THUS CAN BE MADE BY PLOTTING $1/\Theta$ VS $1/P$ AND CHECKING FOR LINEARITY. THIS YIELDS REASONABLE LINEARITY FOR $\underline{T \gtrsim 450\,K}$ AND $\underline{\Theta \lesssim 0.25\,ML}$, ALTHOUGH 563 K SHOWS STRONG DEVIATIONS FOR HIGH PRESSURES.

↓

[25] (a) As $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^3$

$2p^2_{1/2}\ \ 2p^4_{3/2}\ \ 3p^2_{1/2}\ \ 3p^4_{3/2}\ \ 3d^4_{3/2}\ \ 3d^6_{5/2}$

E_b's : 11867 1527 1359 1323 205 146 141 42 42 $\boxed{?\ \ ?}$

NO, E_b's FOR 4s AND 4p ARE NOT SHOWN. THESE ARE VALENCE e^-'s, SO E_b ALWAYS ~ 0 – 30 eV AND OFTEN NOT SHOWN IN TABLES.

(b) $E_{kin} = h\nu - E_b(k)$

$= 2{,}000\ eV - E_b(k) =$

PHOTO e^- PEAKS AT:

473 eV – 2s
641 eV – $2p_{1/2}$
677 eV – $2p_{3/2}$
1,795 eV – 3s
1,854 eV – $3p_{1/2}$
1,859 eV – $3p_{3/2}$
1,958 eV – $3d_{3/2}$
1,958 eV – $3d_{5/2}$
~ 1,970 – 2,000 —— 4s + 4p VALENCE

(c) $h\nu(K\alpha_1) = E_b(As, 1s) - E_b(As, 2p_{3/2}) = 10{,}543.4\ eV$ — TABLE 10,543.7 eV

$h\nu(K\alpha_2) = E_b(As, 1s) - E_b(As, 2p_{1/2}) = 10{,}507.9\ eV$ — 10,508.0 eV

$h\nu(L\beta_1) = E_b(As, 2p_{1/2}) - E_b(As, 3d_{3/2}) = 1{,}317.4\ eV$ — 1,317.0 eV

EXCELLENT AGREEMENT

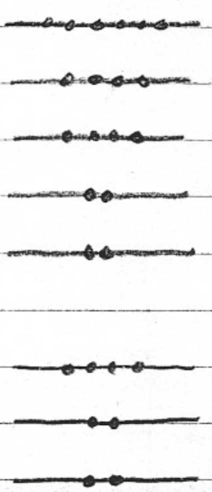
[2.5] (d) MOST ACCURATE ENERGY FORMULA IS:

(CONT'D)
$$E_{kin}(L_iM_kM_l) \geq \underset{\substack{(As)\\ z}}{E_b(L_i)} - 1/2\Big(\underset{\substack{(As)\\ z}}{E_b(M_k)} + \underset{\substack{(Se)\\ z+1}}{E_b(M_k)}\Big) - \tfrac{1}{2}\Big(\underset{\substack{(As)\\ z}}{E_b(M_l)} + \underset{\substack{(Se)\\ z+1}}{E_b(M_l)}\Big)$$

AND CRUDE RELATIVE INTENSITY ESTIMATE IS

$$\text{INT. } (L_i M_k M_l) = (\underbrace{2j_i+1)(2j_k+1)(2j_l+1}_{\text{NO. } e^-\text{'S IN EACH LEVEL}})$$

LEVELS INVOLVED ARE:



	As E_b(eV)	Se E_b(eV)
M_5 (6)	41.7	54.6
M_4 (4)	41.7	55.5
M_3 (4)	141.2	160.7
M_2 (2)	146.2	166.5
M_1 (2)	204.7	229.6
L_3 (4)	1326.6	1433.9
L_2 (2)	1359.1	1473.3
L_1 (2)	1527.0	1652.0

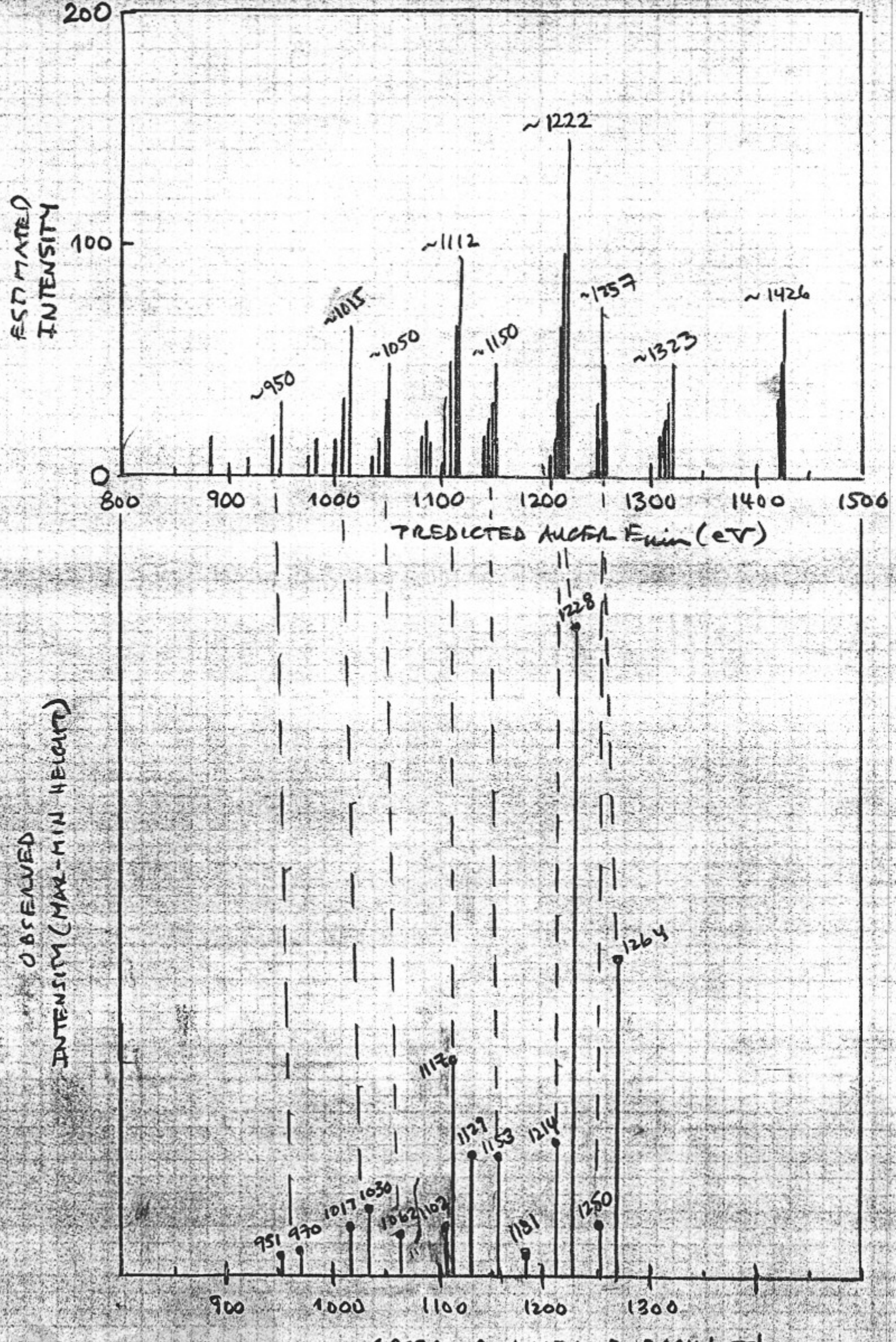
WITH A LOT OF ARITHMETIC, THE RESULTING 45 ALLOWED TRANSITIONS, ENERGIES AND INTENSITIES ARE:

	M_kM_l	L_1	INT.	L_2	INT.	L_3	INT.
$k,l =$	1, 1	1089.0	8	920.0	8	885.0	16
	1, 2	1148.0	8	979.0	8	944.0	16
	1, 3	1154.5	16	985.5	16	950.5	32
	1, 4	1256.5	16	1087.5	16	1052.5	32
	1, 5	1257.5	24	1088.5	24	1053.5	48
	2, 2	1207.0	8	1038.0	8	1003.0	16
	2, 3	1213.5	16	1044.0	16	1117.5	32
	2, 4	1315.5	16	1146.5	16	1112.5	32
	2, 5	1316.5	24	1147.5	24	1016.0	48
	3, 3	1220.0	32	1051.0	32	1118.0	64
	3, 4	1322.0	32	1153.0	32	1220.0	64
	3, 5	1323.0	48	1154.0	48	1222.0	96

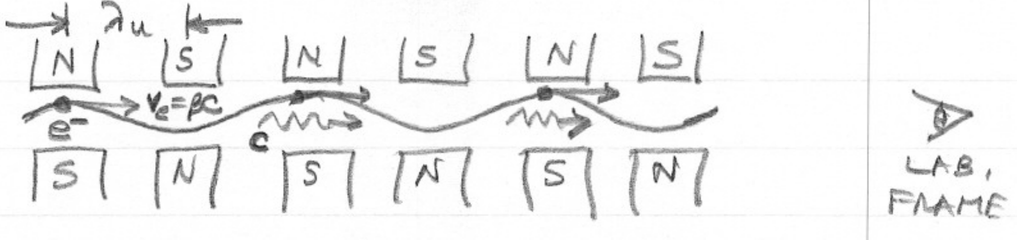
M_4M_5	L_1	INT.	L_2	INT.	L_3	INT.
4,4	1424.0	32	1255.0	32	1220.0	64
4,5	1425.0	48	1256.0	48	1221.0	96
5,5	1426.0	72	1257.0	72	1222.0	144

THE CORRELATION OF EXPT. & THEORY IS SHOWN ON THE NEXT PAGE, AND IT IS VERY GOOD, WITH ALL MAIN PEAKS/GROUPS OF PEAKS BEING CORRECTLY PREDICTED IN THE CALCULATIONS. THE OBSERVED POSITIONS GENERALLY ~ 5-10 eV HIGHER IN E_{KIN}, WHICH IS ONLY $\lesssim 1\%$ OFF. NOT BAD!

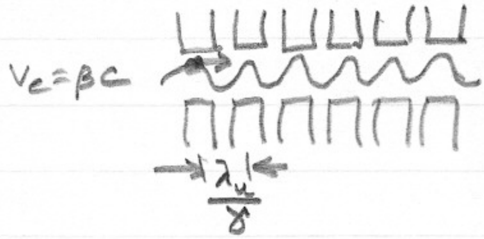
FROM THIS, WE CAN GO ON TO PREDICT THAT, IF THE EXPERIMENTAL SPECTRUM WERE EXTENDED TO 1500 eV, WE WOULD SEE PEAKS AT ~ 1325 - 1370 eV AND 1430 - 1435 eV.


200
100
0
ESTIMATED INTENSITY
~950
~1015
~1050
~1112
~1150
~1222
~1257
~1323
~1426
800
900
1000
1100
1200
1300
1400
1500
PREDICTED AUGER Emin (eV)
OBSERVED INTENSITY (MAX-MIN HEIGHT)
1228
1264
1110
1129
1153
1214
1017
1030
951
970
1062
1102
1181
1250
900
1000
1100
1200
1300
OBSERVED AUGER ENERGY (eV)

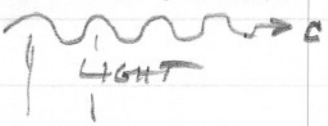
[3.1] (a)



IN ELECTRON FRAME: LORENTZ CONTRACTION ALONG e⁻ MOTION



=> OSCILLATING DIPOLE AT $\frac{\beta c}{(\lambda_u/\gamma)} = \frac{\gamma\beta c}{\lambda_u}$



$\Updownarrow$

FUNDAMENTAL FREQUENCY $= \nu_{e,1}$

IN LAB. FRAME: LIGHT IS DOPPLER SHIFTED TO HIGHER ν_1

$$\nu_1 = \nu_{e,1} \underbrace{\frac{[1+\beta]^{1/2}}{[1-\beta]^{1/2}}}_{\text{RELATIVISTIC DOPPLER FORMULA}} = \frac{\gamma\beta c}{\lambda_u}\frac{[1+\beta]^{1/2}}{[1-\beta]^{1/2}} \overset{\uparrow}{=} \frac{\beta c}{\lambda_u}\left(\frac{1}{1-\beta}\right)$$

$$\gamma = \frac{1}{\sqrt{1-\beta^2}} = \frac{1}{\sqrt{1+\beta}\sqrt{1-\beta}}$$

BUT $\beta < 1$ BUT VERY CLOSE TO IT, SO THIS BECOMES

$$\nu_1 = \frac{c}{\lambda_u}\left[2\gamma^2\right]$$

AND $$\boxed{\lambda_1 = \frac{c}{\nu_1} = \frac{\lambda_u}{2\gamma^2}}$$

(b) NEXT PAGE

[3.1] (b) HIGHER HARMONICS OCCUR AT $\frac{\lambda_1}{n}$ AND CANNOT BE EXPLAINED AS SIMPLY, SINCE WE MUST CONSIDER TRANSVERSE e^- MOTION + HIGHER HARMONICS IN IT, WHICH INTRODUCE ADDITIONAL PATH-LENGTH DIFFERENCE:

NOTE: (ACTUAL MOTION ⊥ PAGE)

- 2ND HARMONIC IMPLIES DEFLECTIONS THAT ARE 1/2 THE TIME OUT OF PHASE WITH MAGNETIC FORCES. ETC. FOR 4TH, 6TH, -- ∴ THESE HARMONICS ARE WEAKER ALONG AXIS.
- 3RD, 5TH, 7TH HARMONICS ARE ALWAYS IN PHASE WITH MAGNETIC FORCES, + ∴ ARE STRONGER ALONG AXIS.

(SEE ATTWOOD FOR MORE QUANTITATIVE DISCUSSION.)

See following pages of explanation from A. Kaiser

- Additional comments on undulator harmonic brightness:

- From Dr. Alexander Kaiser, Fadley Group, October, 2010:

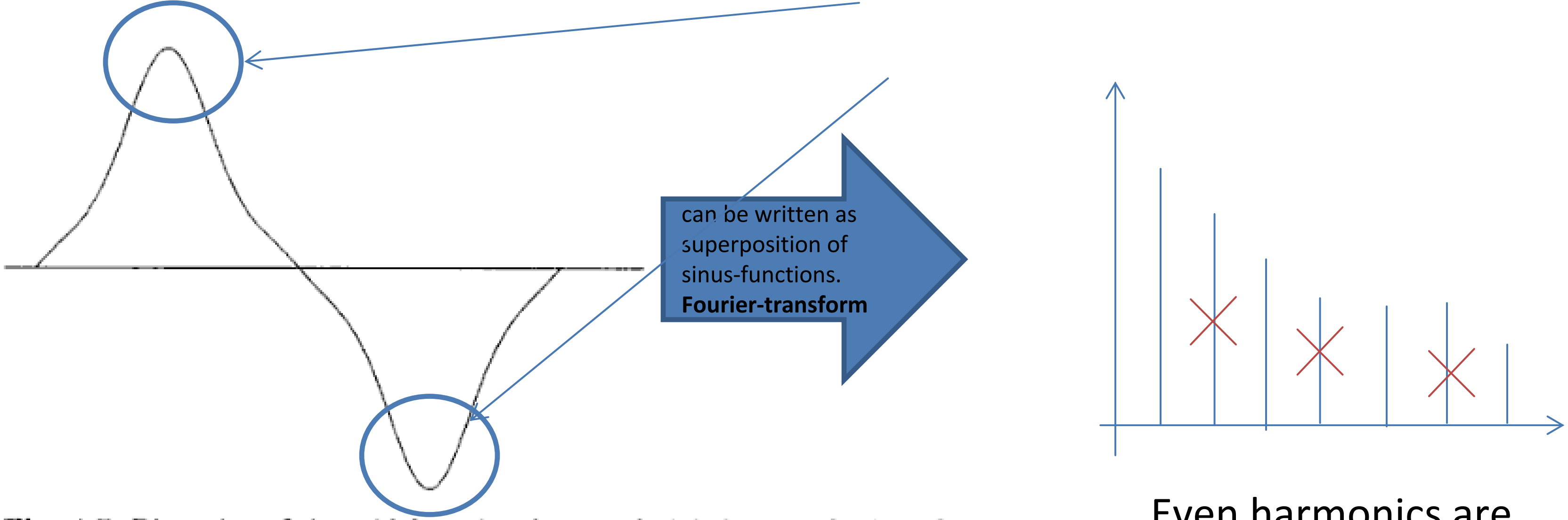
- I think the reason is a simple symmetry argument regarding the electron trajectories. It has nothing to do with interference from neighboring curves of the electron trajectories, but with harmonics in the electron motion itself. A basic sinusoidal trajectory of the electrons would only give the fundamental frequency.
-

- Within the magnet array the electrons are periodically accelerated/decelerated in longitudinal and transverse direction. The transversal acceleration follows the profile of the magnetic field so it repeats every undulator period while the longitudinal acceleration has the double frequency of that (maximum longitudinal velocity at the reversal points of the transverse motion - twice within one undulator period). This leads to periodic Lorentz contraction in longitudinal direction. Thus, in the restframe of the electron the sinusoidal motion is distorted (see attachment). This distorted trajectory can be written as a superposition of different sinusoidal trajectories - the fundamental and some higher harmonics of that. However, the distorted path is symmetric around its maxima - an even harmonic would never have that symmetry (see attachment) and thus only odd harmonics are allowed. Another argument would be that you want to have the trajectories to be invariant under inversion of the electron direction which wouldn't be possible considering even harmonics. So, one can consider the electron trajectory to be a superposition of sinusoidal trajectories with fundamental wavelength and (only) odd harmonics of that - leading to the emission of odd harmonics along the undulator axis. However, due to that longitudinal acceleration you observe even harmonics in off-axis direction!
-

Why only odd harmonics on axis?

Generation of harmonics not due to interference but due to the existence of harmonics in the motion of the electrons.

Transversal relativistic acceleration of the electron leads to a periodic contraction in longitudinal direction. Contraction is high when electron moves parallel to the axis and lowest when the transverse component is maximum.



can be written as superposition of sinus-functions. **Fourier-transform**

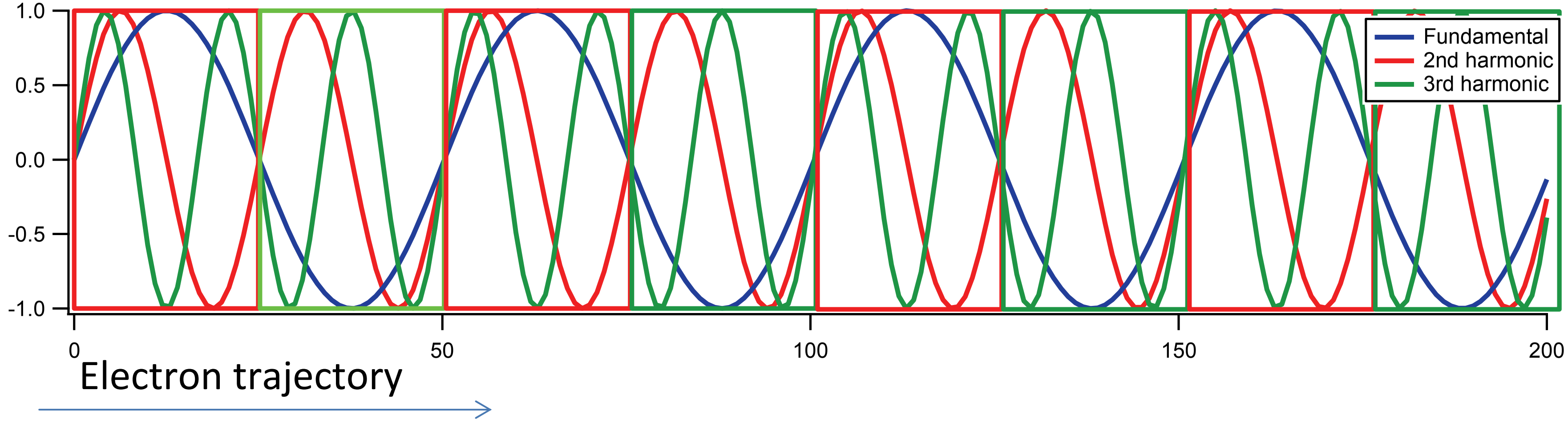
Fig. 4.7. Distortion of sinusoidal motion due to relativistic perturbation of transverse motion

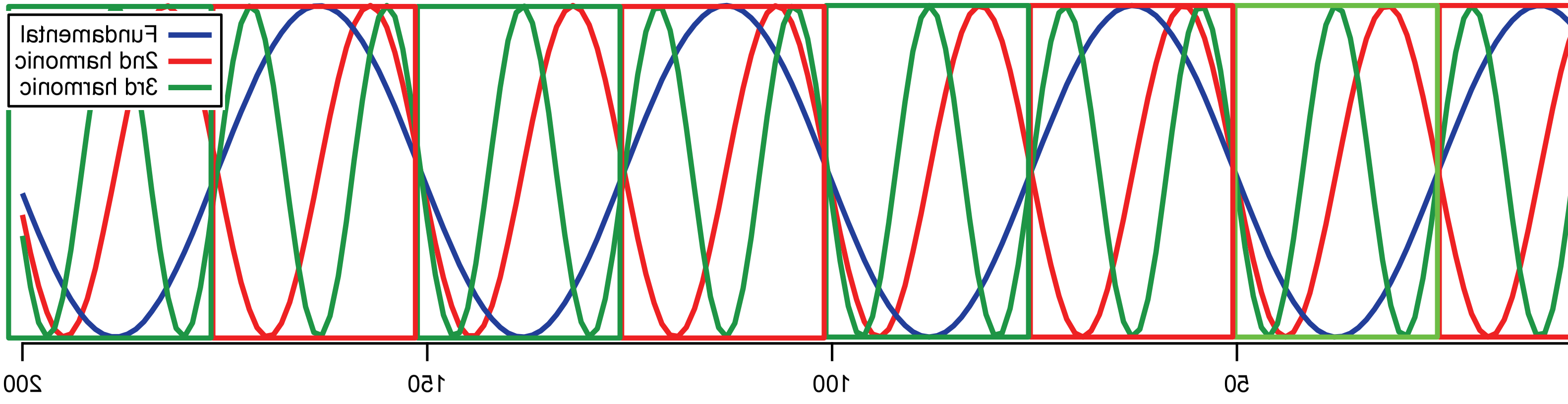
From: Wiedemann, Synchrotron radiation, Springer

Even harmonics are not possible due to symmetry reasons

Invariance under inversion of electron trajectory

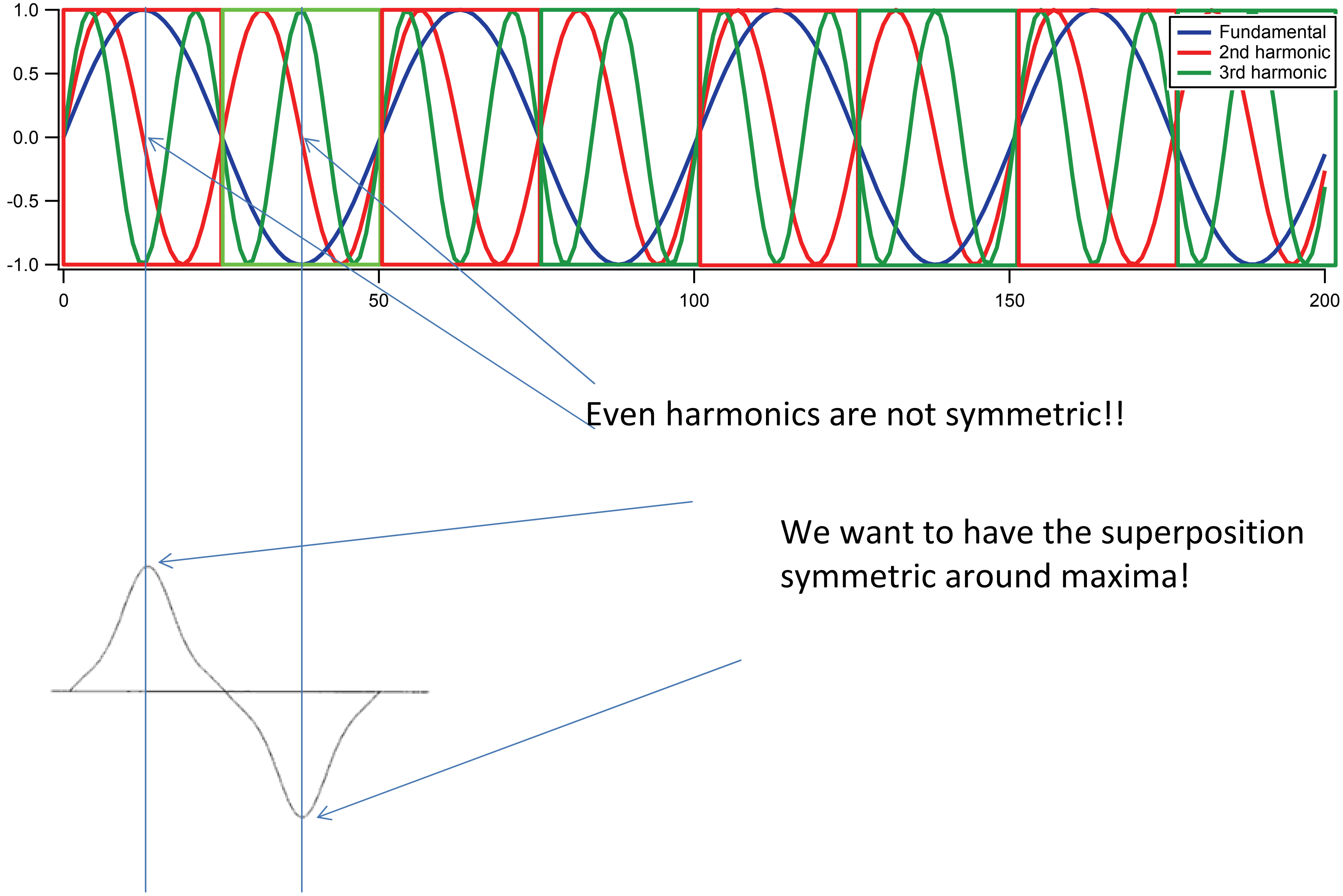
Red/Green magnet arrays





Inverted direction of electron motion
Only odd harmonics follow same trajectory!

Another argument

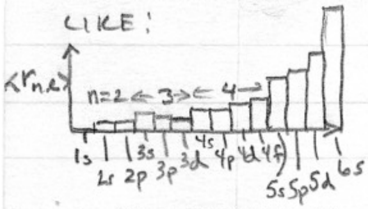


Even harmonics are not symmetric!!

We want to have the superposition symmetric around maxima!

[3.2] (a) Shell structure <u>is</u> evident in clustering of mean radii $\langle r_{n\ell} \rangle$ for each n. Each n ≃ "shell" of e^- charge.

BAR PLOT LIKE:

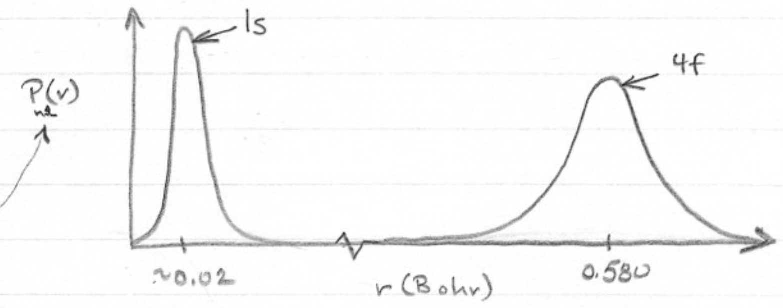


~ STAIRSTEPS, ONE FOR EACH n

(b) Average separation between 1s and 2s orbitals is smaller than that between 1s and 3s orbitals. Therefore,

$$\boxed{J_{1s,2s} > J_{1s,3s}},$$

(c) The 1s and 4f radial probability distributions are roughly:



NOTE
IMP. GENERAL
RULES HERE:

⊙ $R_{n\ell}(r)$ HAS $n-\ell-1$ NODES.

⊙ ∴ $P_{n\ell}(r) = r^2 R_{n\ell}(r)$ HAS $n-\ell$ <u>MAXIMA</u>

RADIAL PROBAB. DENSITY

Overlap is ∴ very small, and

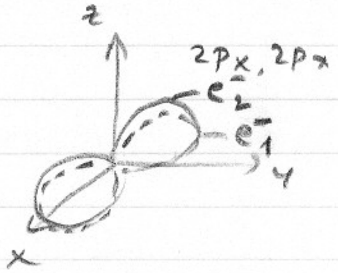
$$\boxed{\bar{K}_{1s,4f} \approx 0 < \bar{\bar{J}}_{1s,4f}}$$

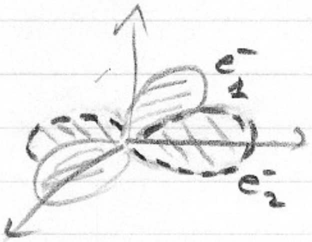
(d) Two electrons in the same orbital will have a smaller average separation than two electrons with the same principal quantum no. but different l values. I.e., different l values have different nodal structure and ∴ less overlap. So,

$$\boxed{\bar{J}_{4d,4d} > \bar{J}_{4d,4f}}.$$

↓

(e) Two e^- in $2p_x$ have maximum spatial overlap, whereas $2p_x$ and $2p_y$ are ⊥ in space: Thus, $\frac{1}{r_{12}}$ is larger in first case, and $\boxed{J_{2p_x,2p_x} > J\,2p_x,2p_y}$

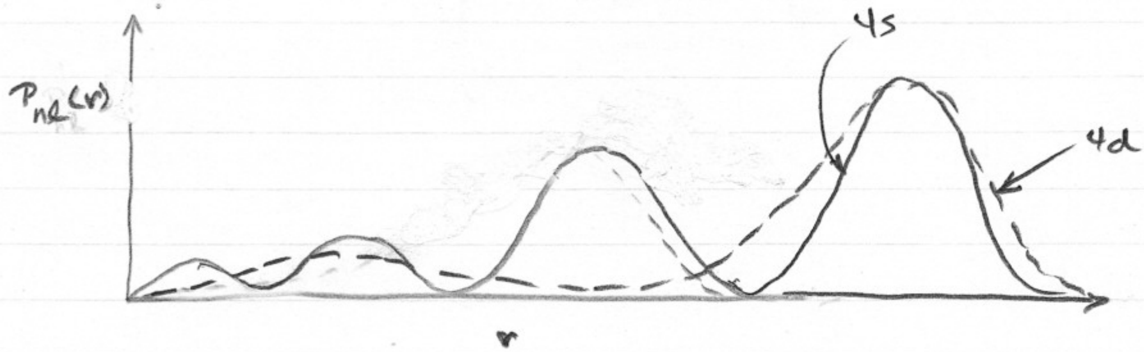




(f) $2p_x$ e^-'s are confined to a smaller region of space than $3p_x$ e^-'s, so $\frac{1}{r_{12}}$ will be larger and

$$\boxed{J_{2p_x,2p_x} > J_{3p_x,3p_x}}$$

(g) Note that 4s electrons have slightly smaller $\langle r \rangle$ than 4d electrons. Also, the 4s radial probability distribution has extra lobes near the nucleus. There is only one such lobe for 4d.

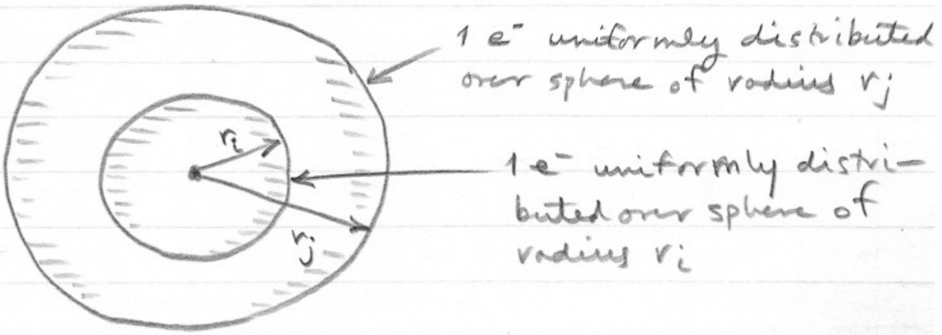


Thus, part of the 4s probability distribution penetrates much closer to the nucleus and the inner shell screening is less effective for 4s. So,

$$\boxed{\text{4s sees greater effective nuclear charge.}}$$

This greater effective nuclear charge is also reflected in the binding energy difference $E_b(4s) > E_b(4d)$. It is also apparent in screening parameters for Slater type orbitals (see q.m. book on atoms).

(h) In the limit that orbital charge distributions are spherically symmetric and relatively little overlapping, we can approximate two different distributions as spherical shells of charge:



Thus, the coulomb integral between them, which in general is given by

i + j charge densities

$$J_{ij} = \iint \frac{\varphi_i^*(\vec r_1)\varphi_j^*(\vec r_2)\, e^2\, \varphi_i(\vec r_1)\varphi_j(\vec r_2)}{|\vec r_1 - \vec r_2|}\, d^3r_1\, d^3r_2 = \iint \frac{\rho_i(\vec r_1)\,\rho_j(\vec r_2)}{|\vec r_1 - \vec r_2|}\, d^3r_1\, d^3r_2$$

can be simplified to:

$$= \underbrace{\frac{e}{4\pi r_i^2}\cdot\frac{e}{4\pi r_j^2}}_{\text{Surface charge densities on spheres}} \iint_{\substack{\text{sphere} \\ i}\ \substack{\text{sphere} \\ j}} \frac{1}{|\vec r_1 - \vec r_2|}\, dS_1\, dS_2$$

From classical e.+m., it is now a simple matter to show that the inner sphere acts on the outer sphere exactly like a point charge situated at the origin. It generates an electrostatic potential of $V = e/r$ outside of r_i and this in turn interacts with sphere j to give

$$J_{ij} = \underbrace{\frac{e^2\,(esu^2)}{r_j\,(cm)}}_{\text{ergs}} = \underbrace{\frac{1}{r_j\,(a.u.)}}_{\text{a.u.}}$$

1 a.u. = 27.21 eV.

Thus, our estimates for coulomb integrals become

	CLASSICAL	HARTREE-FOCK	RATIO OF CLASSICAL / HF
$J_{1s,4s}$	2.05	2.73	0.752
$J_{1s,5s}$	0.845	1.08	0.786
$J_{1s,6s}$	0.264	0.326	0.798

Fairly close to HF vals., although classical always < HF due to neglected overlap of orbitals. Classical slightly better for 1s, 6s with lowest overlap. Note that 4s, 5s, and 6s all have radial lobes near 1s, however.

(i) The exchange interaction is uniquely quantum-mechanical, and so, has no classical analogue. It depends on knowing orbitals, ϕ_i, not just charge densities $|\phi_i|^2$. So there is no way to estimate it classically.