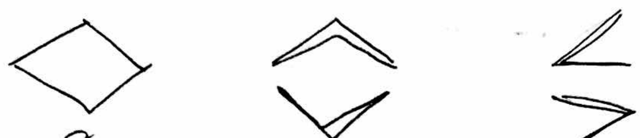
Inclusion of non-coplanar terms

From Note of 2/20/14

we have the following combinatorics for planar terms



8 (u_1)   8 (u_2)   8 (u_3)

– total 24 (arrange 4 distinct objects ($q_1 \bar{q}_1\, q_2 \bar{q}_2$), 4!

all of them contribute to

$$u(\alpha_{12}) |\rho_{q_1}|^2 |\rho_{q_2}|^2$$

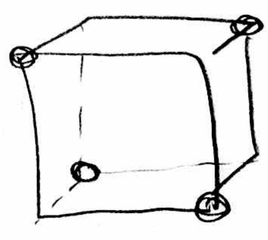
in the code we drop factor 8.

Non coplanar diagram has 4 really distinct $\bar{q}$'s, $\sum_{i=1}^{4} q_i = 0$. Same combinatorics gives 24 pos. for each set of 4.

For FCC, reciprocal is BCC, and hence $\bar{q}$'s are corners of a cube = 2× tetrahedron.

2 sets of q's.

Hence, full interaction energy is



$$\sum_i \underbrace{\left(4u_1(0) + 2u_3(0)\right)}_{3\cdot 2\tilde{u}(0)} |\rho_i|^4$$

$$+ 8\sum_{i<j} \underbrace{\left(u_1(d_{ij}) + u_2(d_{ij}) + u_3(d_{ij})\right)}_{3\tilde{u}(d)} |\rho_i|^2 |\rho_j|^2$$

convention in code

$$+ 24 \sum_{\substack{\text{set}\\ \text{of}\\ 4}} v_4 \, \rho_1 \rho_2 \rho_3 \rho_4$$

For symmetric states can choose $|\rho_i| = a$.
the sign of last term can be chosen at will,
includes both electronic contribution and
"Coulomb" c

Full interaction is, for symmetric states

$$F_{int} = 2\cdot 3\,\tilde{u}(0) \sum_i |\rho_i|^4$$

$$+ 3\cdot 4 \sum_{i\neq j} \tilde{u}(d_{ij}) |\rho_i|^2 |\rho_j|^2$$

$$+ 24 \sum_{\text{sets } 4} v_4 \, \rho_1 \rho_2 \rho_3 \rho_4$$

$$= 3\cdot 4 \left(N \frac{\tilde{u}(0)}{2} + N \sum_{i\neq 0} \tilde{u}(d_{i0}) - 2 n_4 |v_4| \right) a^4$$

(for FCC $n_4 = 2$)

with Coulomb

$$\tilde{u} \to \tilde{u} + c$$

$$v_4 \to v_4 + c$$

Energy

$$F = rNa^2 + (\qquad)a^4 , \quad a^2 = -\frac{rN}{2(\quad)}$$

$$F = -\frac{rN^2}{2\underbrace{(\qquad)}_{\text{Denominator}}}$$

Denominator

$$\left(\sum_{i\neq 0}\tilde{u}(\alpha_{i0}) + \frac{\tilde{u}_0}{2}\right)\frac{1}{N} - \frac{2n_4}{N^2}|v_4|$$

with Coulomb

$$+ \; C\left(1-\frac{1}{2N}\right) - \frac{2n_4}{N^2}|v_4+C|$$

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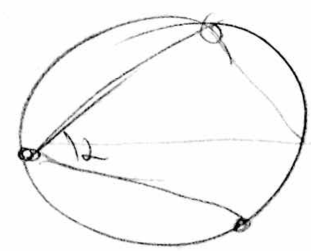
1.75 $\quad \cos\alpha = 1/3$



$$k_F\sqrt{2(1+\cos\alpha)} = k_F\sqrt{8/3}$$

$$2k_F \cancel{q_0} \cos\frac{\alpha}{2} = q_0$$

$$2k_F\sqrt{\frac{1+\cos\alpha}{2}} = q_0$$