

**Marder 3.2**

```
> restart;  
> with(LinearAlgebra):  
> assume(a,positive);assume(c,positive);  
> a1:=<a,0,0>;  
al := 
$$\begin{bmatrix} a \\ 0 \\ 0 \end{bmatrix}$$
  
  
> a2:=<a/2,a*sqrt(3)/2,0>;  
a2 := 
$$\begin{bmatrix} \frac{1}{2} a \\ \frac{1}{2} a\sqrt{3} \\ 0 \end{bmatrix}$$
  
  
> a3:=<0,0,c>;  
a3 := 
$$\begin{bmatrix} 0 \\ 0 \\ c \end{bmatrix}$$
  
  
> b1:=2*Pi*CrossProduct(a2,a3)/DotProduct(a1,CrossProduct(a2,a3));  
b1 := 
$$\begin{bmatrix} \frac{2\pi}{a} \\ -\frac{2\pi\sqrt{3}}{3a} \\ 0 \end{bmatrix}$$
  
  
> b2:=2*Pi*CrossProduct(a3,a1)/DotProduct(a1,CrossProduct(a2,a3));  
b2 := 
$$\begin{bmatrix} 0 \\ \frac{4\pi\sqrt{3}}{3a} \\ 0 \end{bmatrix}$$
  
  
> b3:=2*Pi*CrossProduct(a1,a2)/DotProduct(a1,CrossProduct(a2,a3));
```

$$b3 := \begin{bmatrix} 0 \\ 0 \\ \frac{2\pi}{c\sim} \end{bmatrix}$$

b2 is 09 degrees clockwise from a1 and 30 degrees clockwise from a2. But since there is an equivalent lattice point in the original real space lattice every 60 degrees, we can equally well consider this lattice as rotated by 90 degrees - 30 degrees = 60 degrees from the original lattice. q.e.d.

## Part B.

```
> v2:=<a/2,a/(sqrt(3)*2),c/2>;
```

$$v2 := \begin{bmatrix} \frac{1}{2} a\sim \\ \frac{1}{6} a\sim \sqrt{3} \\ \frac{1}{2} c\sim \end{bmatrix}$$

```
> G:=n1*b1+n2*b2+n3*b3;
```

$$G := \begin{bmatrix} \frac{2 n1 \pi}{a\sim} \\ -\frac{2 n1 \pi \sqrt{3}}{3 a\sim} + \frac{4 n2 \pi \sqrt{3}}{3 a\sim} \\ \frac{2 n3 \pi}{c\sim} \end{bmatrix}$$

```
> tmp1:=DotProduct(G,v2);
```

$$tmp1 := \pi \overline{n1} + \frac{1}{6} \left( \frac{2 n1 \pi \sqrt{3}}{3 a\sim} + \frac{4 n2 \pi \sqrt{3}}{3 a\sim} \right) a\sim \sqrt{3} + \pi \overline{n3}$$

```
> simplify(%);
```

$$\frac{1}{3} \pi (3 \overline{n1} - \overline{n1} - 2 \overline{n2} + 3 \overline{n3})$$

I do not know why the above does not simplify the two n1 terms.

```
> tmp2:=1+exp(I*tmp1);
```

$$tmp2 := 1 + e^{\left( I\left( \pi \overline{n1} + \frac{1}{6} \cdot \frac{2 n1 \pi \sqrt{3}}{3 a_{\sim}} + \frac{4 n2 \pi \sqrt{3}}{3 a_{\sim}} a_{\sim} \sqrt{3} + \pi \overline{n3} \right) \right)}$$

> F:=tmp2\*Conjugate(tmp2);

$$F := \left( 1 + e^{\left( I\left( \pi \overline{n1} + \frac{1}{6} \cdot \frac{2 n1 \pi \sqrt{3}}{3 a_{\sim}} + \frac{4 n2 \pi \sqrt{3}}{3 a_{\sim}} a_{\sim} \sqrt{3} + \pi \overline{n3} \right) \right)} \right) Conjugate \left( 1 + e^{\left( I\left( \pi \overline{n1} + \frac{1}{6} \cdot \frac{2 n1 \pi \sqrt{3}}{3 a_{\sim}} + \frac{4 n2 \pi \sqrt{3}}{3 a_{\sim}} a_{\sim} \sqrt{3} + \pi \overline{n3} \right) \right)} \right)$$

>

q.e.d.

### Part c.

Extinction occurs when the exponential term is -1. This occurs when the argument of the exponential is an odd multiple of Pi,

that is when  $[2(n1+n2)+3n3] = 3 * (\text{an odd integer})$ .