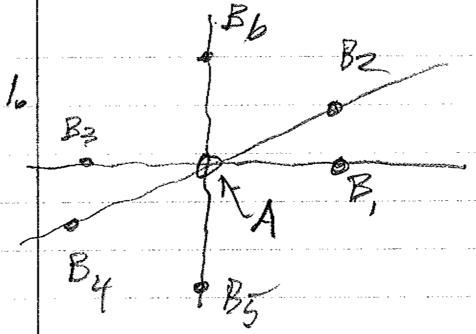
PHY 240A MidTerm #2 Solutions

1. 

$$\begin{array}{c|ccccccc} & A & B_1 & B_2 & B_3 & B_4 & B_5 & B_6 \\ \hline A & \varepsilon_A & t & t & t & t & t & t \\ B_1 & t & \varepsilon_B & & & & & \\ B_2 & t & & \varepsilon_B & & \text{zero} & & \\ B_3 & t & & & \varepsilon_B & & & \\ B_4 & t & \text{zero} & & & \varepsilon_B & & \\ B_5 & t & & & & & \varepsilon_B & \\ B_6 & t & & & & & & \varepsilon_B \end{array} = H$$

$t_{AB} \equiv t$ A-B hopping

(It would be simple to add B-B near neighbor hopping.)

2. The def'n of WF is $W(r-R) = \frac{1}{N}\sum_k e^{-ik\cdot R}\psi_k(r) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} e^{-ik\cdot R}\psi_k(r)\,dk.$

Substituting: $W(r-R) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dk\, e^{-ikR}\sum_{R'} e^{ikR'}\phi(r-R')$

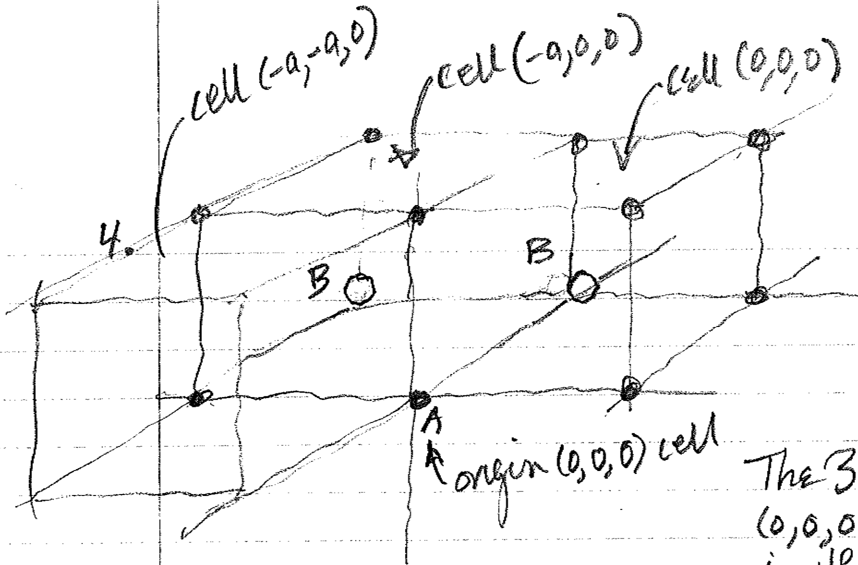
$= \sum_{R'}\phi(r-R')\frac{a}{2\pi}\frac{1}{-ik(R-R')}e^{-ik(R-R')}\Big|_{k=-\pi/a}^{k=\pi/a}$ If $R\neq R'$

But $R=ma$, $R'=na$ for some integers m,n so $\rightarrow e^{-i(m-n)\pi} - e^{i(m-n)\pi}$
$= -2i\sin(m-n)\pi = 0.$

If $R'=R$, the integral is $2\pi/a$. I.e. $\frac{a}{2\pi}\int dk \ldots = \delta_{R,R'}$

$$\boxed{\text{Thus } W(r-R) = \phi(r-R).}$$

3. There are several positives & negatives for each method.
Not try to list here.

4. 

Look at $H_{AB}(k) = \sum_R t_{AB}(R) e^{ik\cdot R}$ first.

What are the $\{\underset{\sim}{R}\}$ vectors for nearest neighbors to (0,0,0)?

The 3 unit cells pictured are (0,0,0), (-1,0,0), (-1,-1,0), the other in this plane is (0,-1,0).

The other 4 are lower by $-a\hat{z}$: (0,0,-1), (-1,0,-1), (-1,-1,-1), (0,-1,-1)

t_{AB}'s are all the same.

Write in order of $R_z = 0$ and $R_z = -a$ pairs, it's systematic

$$t_{AB}\sum_R e^{ik\cdot R} = t_{AB}\Big(\left(1+e^{-ik_z a}\right) + e^{-ik_x a}\left(1+e^{-ik_z a}\right) + e^{-ik_y a}\left(1+e^{-ik_z a}\right)$$
$$+ e^{-i(k_x+k_y)a}\left(1+e^{-ik_z a}\right)\Big)$$
$$= t_{AB}\left[\left(1+e^{-ik_z a}\right)\left(1+e^{-ik_x a}+e^{-ik_y a}+e^{-i(k_x+k_y)a}\right)\right]$$

Can be simplified somewhat but that is a correct result.

Now for $H_{AA}(k) = \sum_R t_{AA}(R)\, e^{ik\cdot R}$. This is easier, as all nearest neighbor A atoms lie in <u>different</u> cells $(\pm1,0,0)$, $(0,\pm1,0)$, $(0,0,\pm1)$

Then $H_{AA}(k) = t_{AA}(2\cos k_x a + 2\cos k_y a + 2\cos k_z a)$

$H_{BB}(k) = t_{BB}($ " " " $)$ by analogy.

$$H(k) = \begin{bmatrix} H_{AA}(k) & H_{AB}(k) \\ H_{AB}^*(k) & H_{BB}(k) \end{bmatrix}.$$

5).

Number of Aluminum atom in one cube cell $\Rightarrow$ 4.

Number of electron per atom $\Rightarrow$ 3

either is OK

$$\text{electron density} = \frac{4\times 3\,\#}{(4\text{Å})^3} = \frac{3}{16}\frac{\#}{\text{Å}^3} = \frac{3}{108.9}\frac{\#}{a_0^3} \quad \text{for } 1a_0 = 0.529\,\text{Å}$$

$$\text{For } N = 2\int^{k_F}\frac{d^3k}{(2\pi)^3} = \frac{k_F^3}{3\pi^2} \Rightarrow k_F = (3\pi^2 n)^{\frac{1}{3}} = \left(3\pi^2\left(\frac{3}{16}\right)\right)^{1/3}\text{Å}^{-1} \approx 6^{1/3}\,\text{Å}^{-1} \approx 1.8\,\text{Å}^{-1}$$

$$\Rightarrow E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{1}{2}(3\pi^2 n)^{2/3}\cdot\underbrace{\left(\frac{\hbar^2}{m a_0^2}\right)}_{Ha}\cdot a_0^2 = \frac{1}{2}\left(3\pi^2\cdot\frac{3}{108.9}\right)^{2/3}\cdot\frac{a_0^2}{a_0^2}\cdot Ha = 0.43\ Ha.$$

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