MIDTERM I

1.

(A) PICK STANDARD PRIMITIVE VECTORS

$$\vec{a}_1 = L\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)$$

$$\vec{a}_2 = L\left(\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{y}\right)$$

WITH A 2 ATOM BASIS $\{0, a\hat{x}\}$

NOW NEED TO FIGURE OUT HOW L IS RELATED TO A.

FROM GEOMETRY, EASY TO SEE

$$\frac{L}{2} = a\cos 30^\circ = \frac{a\sqrt{3}}{2} \Rightarrow L = \sqrt{3}\,a$$

SO

$$\vec{a}_1 = a\left(\frac{3}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right); \quad \vec{a}_2 = a\left(\frac{3}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}\right)$$

BASIS $\{0, a\hat{x}\}$

(B) (SEE SHEET)

(C) HONEYCOMB CRYSTAL IS TRIANGULAR (HEXAGONAL) LATTICE WITH BASIS. HENCE, RECIPROCAL LATTICE IS TRIANGULAR (HEXAGONAL). (THERE REALLY IS NO HONEYCOMB LATTICE)

TO FIND THE RECIPROCAL LATTICE VECTORS, JUST ADD A THIRD ONE, $\vec{a}_3 = c\hat{z}$ AND USE FORMULA FROM A & M FOR 3-D, BUT KEEP ONLY THE ONES IN PLANE.

$$\Rightarrow \quad \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

FROM PART (A)

$$\vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{3}{2}a & -\frac{\sqrt{3}}{2}a & 0 \\ 0 & 0 & c \end{vmatrix} = -\frac{\sqrt{3}}{2}ac\hat{x} - \frac{3}{2}ac\hat{y}$$

$$\vec{a}_3 \times \vec{a}_1 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ \frac{3}{2}a & \frac{\sqrt{3}}{2}a & 0 \end{vmatrix} = -\frac{\sqrt{3}}{2}ac\hat{x} + \frac{3}{2}ac\hat{y}$$

AND

$$\left(\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3\right) = \begin{vmatrix} \frac{3}{2}a & \frac{\sqrt{3}}{2}a & 0 \\ \frac{3}{2}a & -\frac{\sqrt{3}}{2}a & 0 \\ 0 & 0 & c \end{vmatrix} = -\frac{3\sqrt{3}}{2}a^2 c$$

SO

$$\vec{b}_1 = \frac{2\pi}{a}\left(\frac{1}{3}\hat{x} + \frac{\sqrt{3}}{3}\hat{y}\right)$$

$$\vec{b}_2 = \frac{2\pi}{a}\left(\frac{1}{3}\hat{x} - \frac{\sqrt{3}}{3}\hat{y}\right)$$

(D)

$$S_{\vec{k}} = \sum_{\{BASIS\}_{\vec{d}}} e^{i\vec{k}\cdot\vec{d}}$$

$$\vec{d} = \{0,\ a\hat{x}\}$$

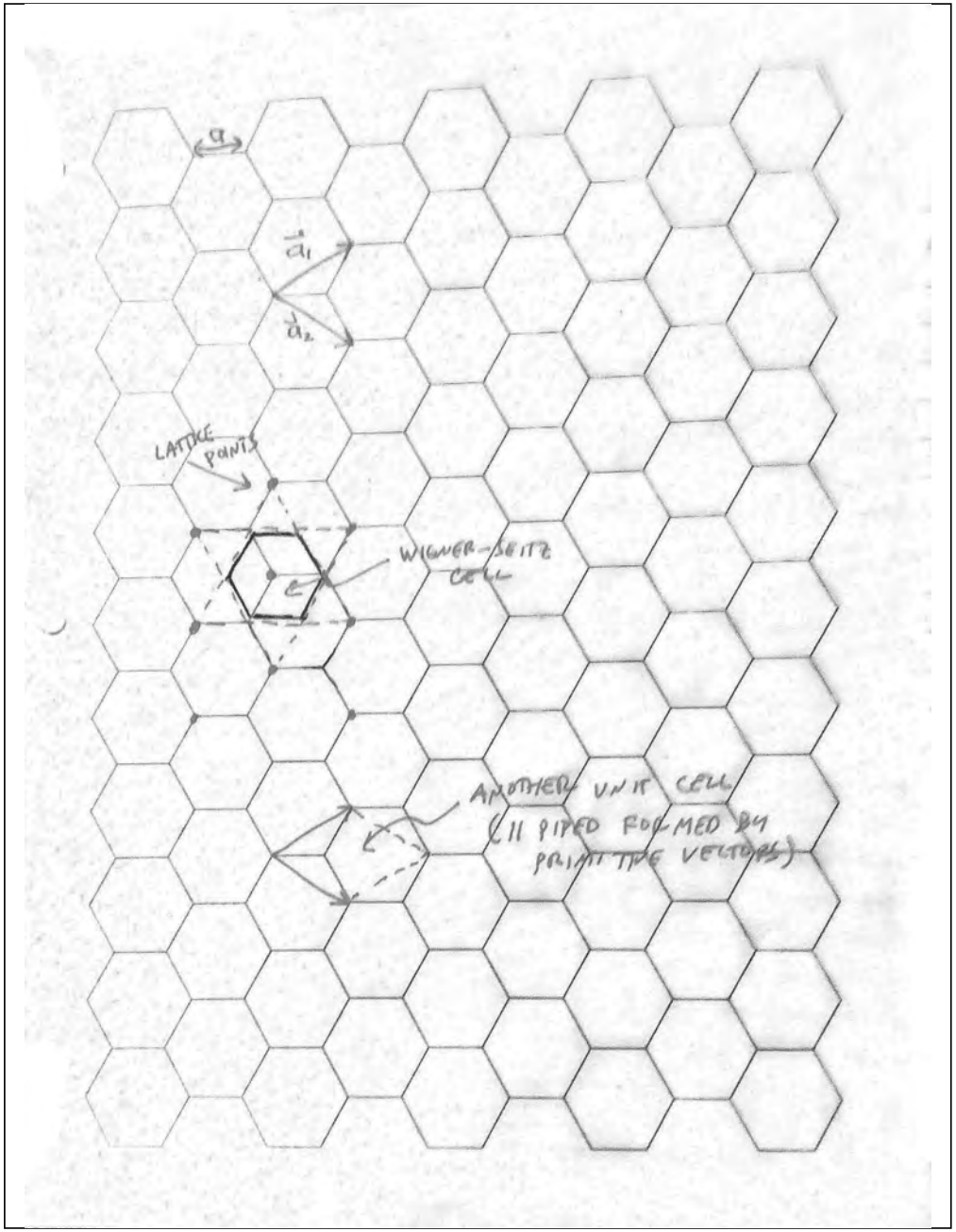
$$\vec{k} = n_1\vec{b}_1 + \vec{n}_2\vec{b}_2$$

SO

$$S_{\vec{k}} = 1 + EXP\left(i\,(n_1+n_2)\frac{2}{3}\pi\right)$$

SO,

$$S_{\vec{k}} = \begin{cases} 2 & (n_1+n_2)\ MOD\,3 = 0 \\ 1+e^{i\frac{2}{3}\pi} & (n_1+n_2)_{MOD\,3} = 1 \\ 1+e^{i\frac{4}{3}\pi} & (n_1+n_2)_{MOD\,3} = 2 \end{cases}$$



DEPENDS ON CHOICE OF PRIMITIVE VECTORS

FOR BCC, a_{bcc} IS THE LENGTH OF THE CUBE (NOT NEAREST NEIGHBOR DISTANCE)

$V_{BCC} = a_{bcc}^3$ WITH $N=2$ ATOMS PER UNIT CELL.

FOR HCP, THERE ARE 2 ATOMS PER UNIT CELL (ONE AT LATTICE POINT AND ONE AT $\frac{a}{\sqrt{3}}\hat{x} + \frac{c}{2}\hat{z}$). FOR HCP, $\frac{c}{a} = \frac{\sqrt{8}}{\sqrt{3}}$.

PRIMITIVE VECTORS hcp:

$$\vec{a}_1 = a_{hcp}\hat{x}$$

$$\vec{a}_2 = a_{hcp}\left(\frac{\hat{x}}{2} + \frac{\sqrt{3}}{2}\hat{y}\right)$$

$$\vec{a}_3 = c\hat{z} = \sqrt{8/3}\, a_{hcp}\hat{z}$$

VOLUME UNIT CELL IS

$$\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} a_{hcp} & 0 & 0 \\ a_{hcp}/2 & \frac{\sqrt{3}}{2}a_{hcp} & 0 \\ 0 & 0 & \sqrt{8/3}\,a_{hcp} \end{vmatrix} = a_{hcp}^3\sqrt{2}$$

SINCE $N_{bcc} = N_{hcp} = 2$,

AND DENSITY IS CONSTANT,

$$\Rightarrow \quad V_{hcp} = V_{BCC} \Rightarrow$$

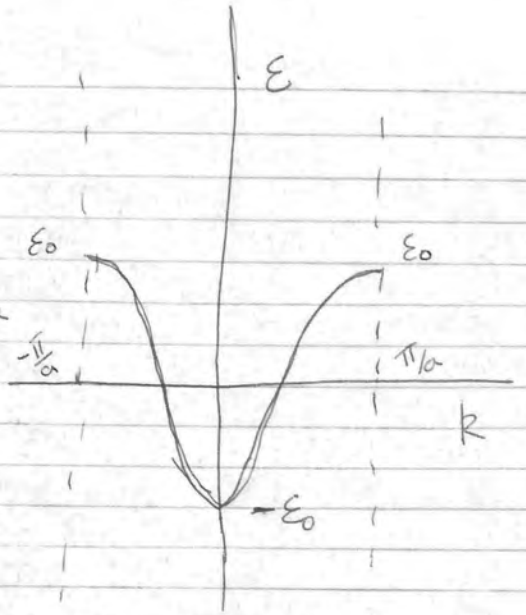
$$a_{hcp}^3 \sqrt{2} = a_{bcc}^3$$

OR $$a_{hcp} = \frac{1}{\sqrt[3]{2}} a_{bcc}$$

FOR $a_{bcc} = 4.23\,\text{Å} \Rightarrow$

$$\boxed{a_{hcp} = 3.77\,\text{Å}}$$

3. (A)



$\varepsilon(k) = -\varepsilon_0 \cos ka$

(B)

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k^2}$$

$$\frac{\partial^2 \varepsilon}{\partial k^2} = \varepsilon_0 a^2 \cos ka$$

SO $$m^* = \left(\frac{\hbar^2}{\varepsilon_0 a^2}\right)\left(\cos ka\right)^{-1}$$

@ $k = 0$, $\boxed{m^* = \frac{\hbar^2}{\varepsilon_0 a^2}}$

AT BZ BOUNDARY $\left(k = \pm \frac{\pi}{a}\right)$ $\boxed{m^* = -\frac{\hbar^2}{\varepsilon_0 a^2}}$

(C) PERIODIC BOUNDARY CONDITIONS $\Rightarrow$

$$\psi_k(0) = \psi_k(L)$$

$$\Rightarrow e^{ikL} = 1 \Rightarrow$$

$$kL = m(2\pi)$$

AND $k = m\frac{2\pi}{L}$ WITH m AN INTEGER

THE NUMBER OF "k" STATES BETWEEN

$k = -\frac{\pi}{a}$ AND $k = +\frac{\pi}{a}$

TELLS US m CAN GO FROM

$$m = -\frac{L}{2a} \ldots\ldots +\frac{L}{2a}$$

SO THERE ARE $2\left(\frac{L}{2a}\right) = \left(\frac{L}{a}\right)$

ALLOWED STATES. IF WE INCLUDE SPIN, WE GET

$$N = \frac{2L}{a} \quad \text{STATES (WITH SPIN)}$$

FOR THE "LINEAR" DENSITY,

$$n = \frac{N}{L} = \frac{2}{a}$$

(D) WE HAVE AT $T=0$

$$N = \sum_{k,s} 1 = 2\left(\frac{L}{2\pi}\right)\int_{-k_f}^{+k_f} dk$$

(SPIN; DENSITY OF STATES IN k-SPACE)

HENCE

$$N = 4\left(\frac{L}{2\pi}\right)k_f \quad \text{SO}$$

$$k_f = \left(\frac{N}{L}\frac{\pi}{2}\right) = n\frac{\pi}{2}$$

$$k_f = n\frac{\pi}{2} \qquad 1\text{-D}$$

(YOU CAN COUNT THE $k=0$ STATE TOO, BUT REMEMBER $k=+\frac{\pi}{a}$ AND $k=-\frac{\pi}{a}$ ARE THE SAME STATE SINCE THEY DIFFER BY A R.L.V.)

So $\boxed{\varepsilon_F = \varepsilon(k_f) = -\varepsilon_0 \cos\left(n\frac{\pi a}{2}\right)}$

(n MUST BE BELOW $n_{MAX} = 2/a$ TO BE IN THE LOWEST BAND

(E) $\underset{\uparrow}{2}\sum_{k} \rightarrow 2\left(\frac{L}{2\pi}\right)\int_{-k}^{k} dk \rightarrow$

SPIN

$2\left(\frac{L}{2\pi}\right)\underset{\uparrow}{2}\int_0^k dk \rightarrow \int_0^{\varepsilon} D(\varepsilon)\,d\varepsilon$

INTEGRATE OVER + k ONLY

So $\underbrace{D(\varepsilon)}_{\text{DENSITY OF STATES IN ENERGY}}\,d\varepsilon = 2\left(\frac{L}{2\pi}\right)2\,dk$

$\underbrace{g(\varepsilon)}_{\text{DENSITY OF STATES / UNIT LENGTH}} = \frac{D(\varepsilon)}{L} = \frac{2}{\pi}\frac{dk}{d\varepsilon}$

$g(\varepsilon) = \frac{2}{\pi}\frac{1}{\left|\frac{d\varepsilon}{dk}\right|}$ $\qquad \frac{d\varepsilon}{dk} = \varepsilon_0 a \sin ka$

So $\boxed{g(\varepsilon) = \frac{2}{\pi\varepsilon_0 a\left|\sin ka\right|}}$

NOTE! ① HAS RIGHT UNITS

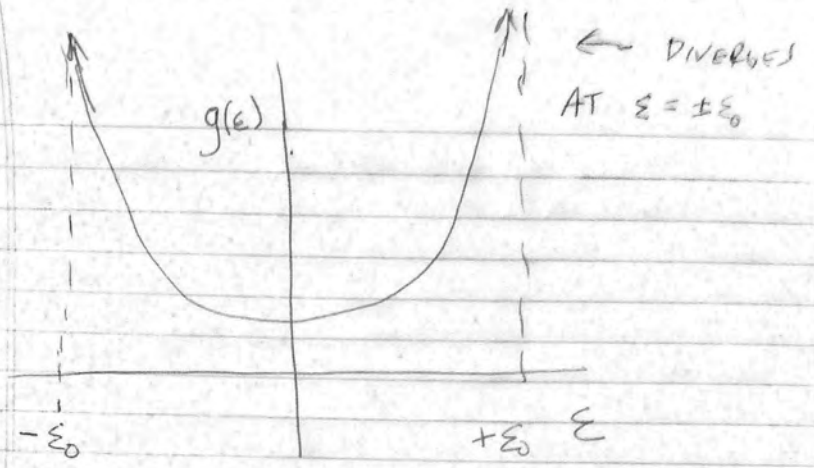
$\frac{1}{\text{ENERGY} - \text{LENGTH}}$

② WE STILL HAVE k IN THE EXPRESSION (I WILL ACCEPT THIS).

REALLY, WE SHOULD ELIMINATE k IN TERMS OF ε

$\left|\varepsilon_0 \sin ka\right| = \sqrt{\varepsilon_0^2 - \varepsilon^2}$

$\boxed{g(\varepsilon) = \frac{2}{\pi a}\frac{1}{\sqrt{\varepsilon_0^2 - \varepsilon^2}}}$



4. THE RECIPROCAL LATTICE VECTORS FOR A BCC CRYSTAL ARE:

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}) \qquad \vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z})$$

PHYS. REV. 129, 2.31

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$$

SO A GENERAL RECIPROCAL LATTICE VECTOR IS:

$n_1 n_2 n_3$ INTEGERS

$$\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$$

$$\vec{G} = \frac{2\pi}{a}\left((n_2+n_3)\hat{x} + (n_1+n_3)\hat{y} + (n_1+n_2)\hat{z}\right)$$

$$n_1, n_2, n_3 \in \mathbb{Z}$$

THE ENERGY BANDS IN THE DIRECTION FROM Γ TO H HAVE A WAVE VECTOR

$$\vec{k} = \frac{2\pi}{a}\left(k\hat{x}\right) \quad \text{WITH } k = 0 \text{ TO } 1$$

THE EMPTY LATTICE ENERGY BANDS ARE

$$\mathcal{E} = \frac{\hbar^2}{2M}\left(\vec{k}+\vec{G}\right)^2$$

WE CAN SCALE THE ENERGY AND WAVEVECTOR TO GET

$$\tilde{\mathcal{E}} = \frac{\mathcal{E}}{\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2} = \left(\left(k_x+n_2+n_3\right)^2 + \left(n_1+n_3\right)^2 + \left(n_1+n_2\right)^2\right)$$

WITH k GOING FROM 0 TO 1
AND $n_1, n_2, n_3 \in \mathbb{Z}$

THE ENERGY THAT IS LOWEST AT THE "H" POINT IS $n_1=n_2=n_3=0$ AND CORRESPONDS TO $\tilde{\mathcal{E}} = 1$ (SCALED)

WE THUS NEED TO GO TO $\tilde{\mathcal{E}}=5$

WE MAKE A TABLE LIKE THE ONE ON PAGE 176.

** NOTE: (n_1, n_2, n_3) ARE THE INTEGERS TIMES b_1, b_2, b_3

NOT $\hat{x}, \hat{y}, \hat{z}$

$\tilde{\mathcal{E}} = \mathcal{E} \Big/ \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2$

BAND	$G\ a/2\pi$	$\tilde{\mathcal{E}}(0,0,0)$	$\tilde{\mathcal{E}}(k_x,0,0)$
1	(0,0,0)	0	$\tilde{k}_x^2$
2	(1,0,0)	2	$2+\tilde{k}_x^2$
3	$(\bar{1},0,0)$	2	
4	(0,1,0)	2	$(\tilde{k}_x+1)^2+1$
5	(0,0,1)	2	"
6	$(0,\bar{1},0)$	2	$(\tilde{k}_x-1)^2+1$
7	$(0,0,\bar{1})$	2	"
8	$(0,1,\bar{1})$	2	$2+\tilde{k}_x^2$
9	$(0,\bar{1},1)$	2	

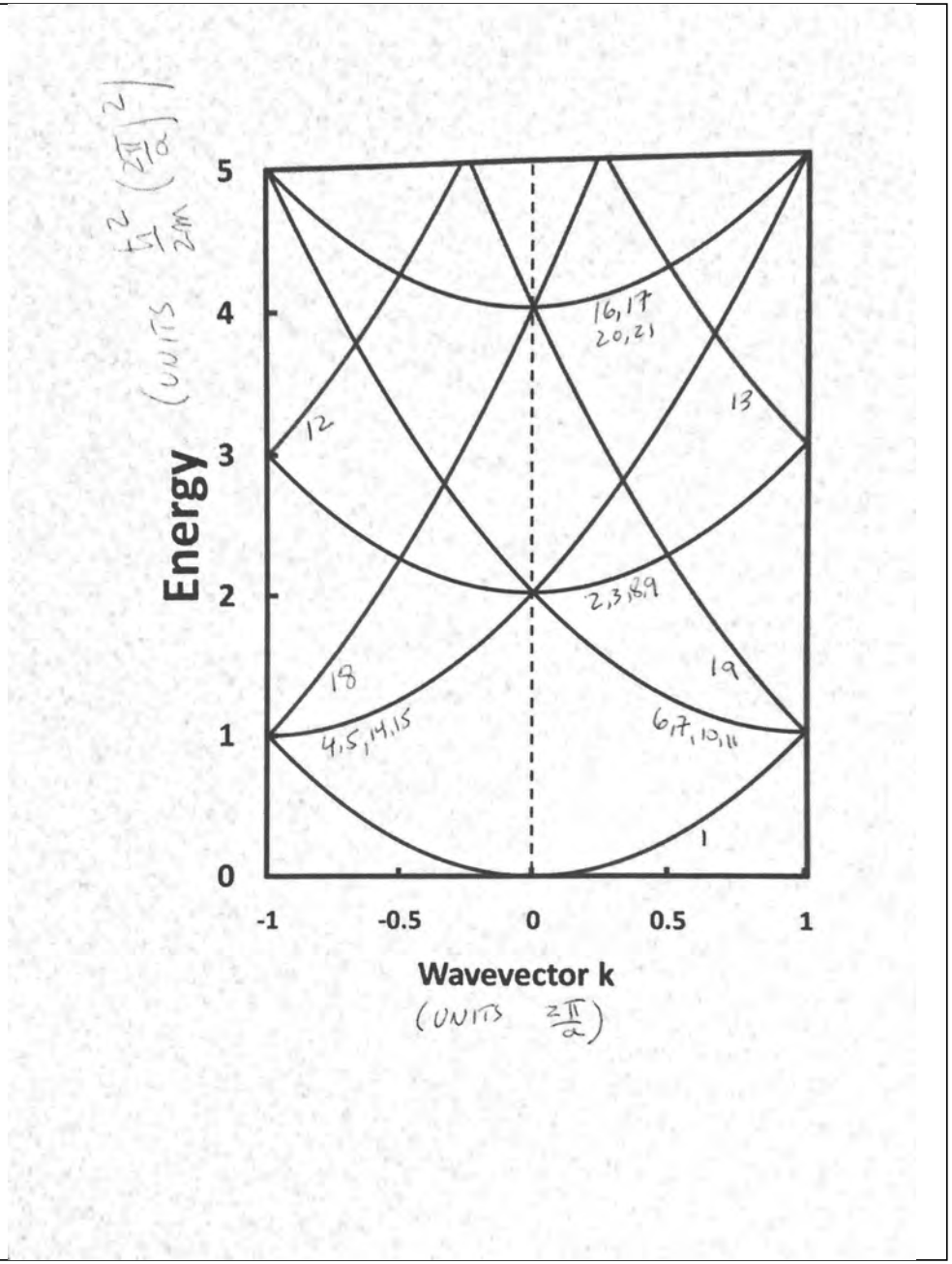
NOTE: k_x IS $k_x/(2\pi/a)$

10	$(1, \bar{1}, 0)$	2	$(\tilde{k}_x - 1)^2 + 1$
11	$(1, 0, \bar{1})$	2	
12	$(0, 1, 1)$	6	$(\tilde{k}_x + 2)^2 + 2$
13	$(0, \bar{1}, \bar{1})$		$(\tilde{k}_x - 2)^2 + 2$
≥ 5	$(1, 1, 0)$	6	$(\tilde{k}_x + 1)^2 + 5$
≥ 5	$(1, 0, 1)$		
	$(\bar{1}, \bar{1}, 0)$		$(\tilde{k}_x - 1)^2 + 5$
	$(\bar{1}, 0, \bar{1})$		
14	$(\bar{1}, 1, 0)$	2	$(\tilde{k}_x + 1)^2 + 1$
15	$(\bar{1}, 0, 1)$	2	
≥ 5	$(1, 1, 1)$	12	$(\tilde{k}_x \pm 2)^2 + 8$
	$(\bar{1}, 1, \bar{1})$		
16	$(1, \bar{1}, 1)$	4	$\tilde{k}_x^2 + 4$
17	$(1, 1, \bar{1})$		
18	$(\bar{1}, 1, 1)$	4	$(\tilde{k}_x \pm 2)^2$
19	$(1, \bar{1}, \bar{1})$	4	
20	$(\bar{1}, 1, \bar{1})$	4	$\tilde{k}_x^2 + 4$
21	$(\bar{1}, \bar{1}, 1)$		

OUCH!! NON-THE LESS, THERE ARE ONLY A FEW PLOTS WE NEED TO DO!

BAND	
1	$\tilde{k}_x^2$
2, 3, 8, 9	$2 + \tilde{k}_x^2$
4, 5, 14, 15	$(\tilde{k}_x + 1)^2 + 1$
6, 7, 10, 11	$(\tilde{k}_x - 1)^2 + 1$
12	$(\tilde{k}_x + 2)^2 + 2$
13	$(\tilde{k}_x - 2)^2 + 2$
16, 17, 20, 21	$\tilde{k}_x^2 + 4$
18	$(\tilde{k}_x + 2)^2$
19	$(\tilde{k}_x - 2)^2$

NOTE THESE ARE < 5 FOR $k_x \neq 0$


Energy
(UNITS $\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2$)
5
4
3
2
1
0
16,17
20,21
13
12
2,3,8,9
19
18
4,5,14,15
6,7,10,11
1
-1
-0.5
0
0.5
1
Wavevector k
(UNITS $\frac{2\pi}{a}$)