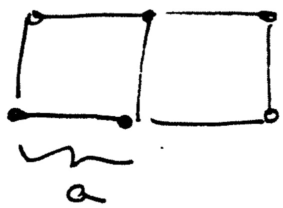
HW 7
Chap. 9

(4) THE REAL SPACE LATTICE IS:

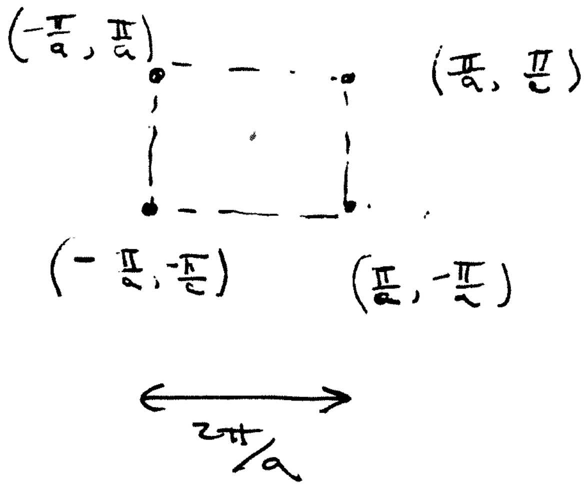
DIRECT:



ETC.

SO THE RECIPROCAL LATTICE IS SQUARE WITH THE LENGTH OF THE SIDE OF THE UNIT CELL $= \frac{2\pi}{a}$

RECIPROCAL:



THE VOLUME OF THE CRYSTAL IS $N_{ION}\, a^2$. THE NUMBER OF ELECTRONS IS $N_{EL} = 2 N_{ION}$.

THE FERMI WAVEVECTOR IS GIVEN BY

$$2\left(\frac{L}{2\pi}\right)^2 \pi k_F^2 = N_{EL} = 2 N_{ION}$$

OR

$$k_F^2 = 4\pi \frac{N_{ION}}{A} = \frac{4\pi}{a^2}$$

$A = N_{ION}\, a^2$

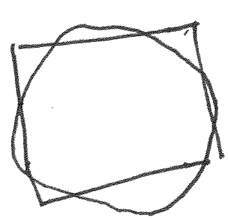
SO

$$k_F = \frac{2\sqrt{\pi}}{a}$$

IN UNITS OF THE HALF WIDTH OF THE UNIT CELL

$$\boxed{\frac{k_F}{(\pi/a)} = \frac{2}{\sqrt{\pi}} = 1.13}$$

(SO k_F GOES JUST OUTSIDE THE FIRST ZONE).



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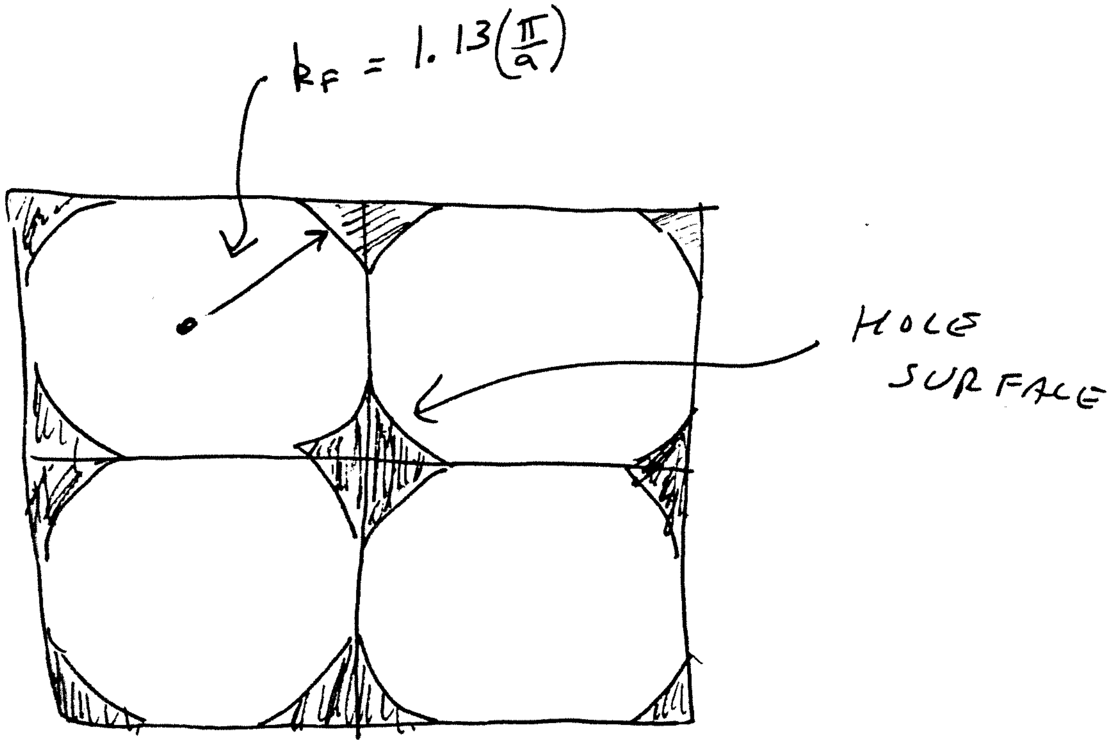
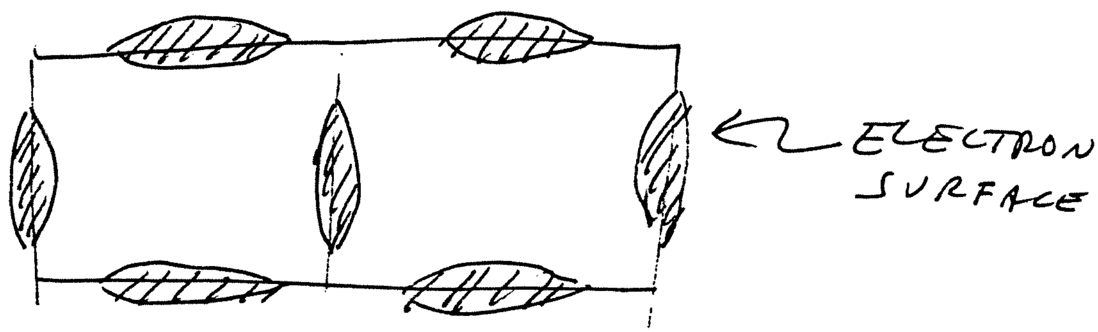
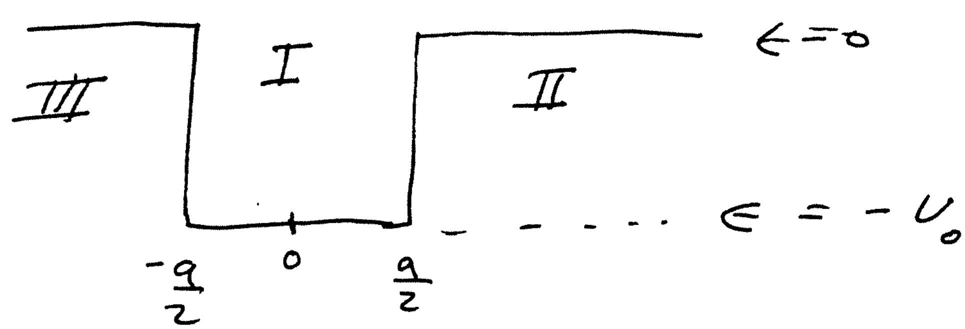




(6) (A) (THIS IS A STANDARD QUANTUM MECHANICAL PROBLEM i.e. SEE MERZBACHER ETC.)



THE S.E. BECOMES:

$$I: \quad \frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + (-V_0)\,\psi(x) = \epsilon\,\psi(x)$$

WHICH HAS SOLUTION

$$\psi(x) = A \cos kx \quad , \quad k = \sqrt{\frac{2m(\epsilon + V_0)}{\hbar^2}}$$

A = CONSTANT TO BE DETERMINED

(NOTE THIS IS THE SOLN. THAT IS SYMMETRIC ABOUT THE MIDPOINT)

II. $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \epsilon\,\psi$$

OR $$\psi = B\,e^{-qx}$$ WITH

$$q = \sqrt{\frac{2mE}{\hbar^2}}$$ (NOTE THIS IS FOR $E < 0$)

III. $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \epsilon\,\psi$$ SO

$$\psi(x) = C\,e^{+qx}$$ WITH

$$q = \sqrt{\frac{-2mE}{\hbar^2}}$$

NOTE: BY SYMMETRY, $B = C$ AND WE NEED ONLY CONSIDER THE BOUNDARY CONDITION AT $x = a/2$. THE B.C. IS

$$\frac{1}{\psi}\frac{d\psi}{dx}$$ IS CONTINUOUS AT $x = a/2$

THIS $\Rightarrow$

~~[illegible]~~ $$\boxed{+k \tan\left(\frac{ka}{2}\right) = q}$$

WITH k & q RELATED TO ε AS ABOVE

(B) IF $|V_0| = 2\hbar^2/ma^2$, THEN

$$k = \sqrt{\frac{2m(\epsilon)}{\hbar^2} + \frac{4}{a^2}}$$

AND $$q = \sqrt{\frac{-2m\epsilon}{\hbar^2}}$$

LET ϵ BE IN UNITS OF V_0 SO THAT

$$k = \frac{2}{a}\sqrt{\epsilon + 1}$$

AND $$q = \frac{2}{a}\sqrt{-\epsilon}$$

SUBSTITUTE INTO ABOVE TO GET

$$\sqrt{\epsilon+1}\ \mathrm{TAN}\left(\sqrt{\epsilon+1}\right) = \sqrt{-\epsilon}$$

OR

$$\boxed{\mathrm{TAN}\left(\sqrt{\epsilon+1}\right) = \sqrt{\frac{-\epsilon}{\epsilon+1}}}$$

THIS CAN NOW BE NUMERICALLY SOLVED.

NOTE HOWEVER, THAT $\boxed{\epsilon = -0.45}$ SOLVES THE <u>EQUATION</u>!!

(MORE SPECIFICALLY:

ϵ	L.H.S	R.H.S
0.44	0.9285	0.8864
0.45	0.9161	0.9045
0.46	0.9036	0.9229

)

(9)

$$w(\vec{r}-\vec{r}_N) = N^{-\frac{1}{2}} \sum_{\vec{k}} EXP(-i\vec{k}\cdot\vec{r}_N)\, \psi_{\vec{k}}(\vec{r})$$

(A)

$$\int dv \quad W^*(\vec{r}-\vec{r}_M)\, W(\vec{r}-\vec{r}_N) =$$

$$\frac{1}{N} \sum_{\vec{k},\vec{k}'} EXP(i\vec{k}'\cdot\vec{r}_M - i\vec{k}\cdot\vec{r}_N) \underbrace{\int dv\, \psi^*_{\vec{k}'}(\vec{r})\, \psi_{\vec{k}}(\vec{r})}_{\delta_{\vec{k}',\vec{k}}}$$

$$= \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}_M-\vec{r}_N)} = \delta_{M,N}$$

(B) $$\omega(x-x_N) = N^{-\frac{1}{2}} \sum_{j=-N+1}^{N} e^{-i\left(\frac{2\pi}{aN} j\, x_N\right)} e^{+i\left(\frac{2\pi}{aN} j\, x\right)} \frac{u_0(x)}{N^{-\frac{1}{2}}}$$

$$= \frac{1}{N}\, u_0(x) \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} e^{+i\left(\frac{2\pi}{aN}(x-x_N)\right) j}$$

$$\approx \frac{u_0(x)}{N} \int_{-\frac{N}{2}}^{\frac{N}{2}} dj\; e^{i\left(\frac{2\pi}{aN}(x-x_N)\right) j}$$

$$= \frac{u_0(x)}{N} \left(\frac{e^{i\left(\frac{2\pi}{aN}(x-x_N)\right) j}}{\frac{2\pi}{aN} i\,(x-x_N)} \right|_{-N/2}^{\frac{N}{2}}$$

$$= \frac{u_0(x)}{N} \frac{\sin \frac{\pi}{a}(x - x_N)}{\frac{\pi}{aN}(x - x_N)}$$

$$= \boxed{u_0(x) \frac{\sin \frac{\pi}{a}(x - x_N)}{\frac{\pi}{a}(x - x_N)}}$$