MIDTERM EXAM

Physics 140B– SPRING 2012

Instructions: Do four of the six problems.

[**1.**] Consider a simple cubic lattice with lattice constant a. That is, the real space lattice vectors are $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, and $\vec{a}_3 = a\hat{z}$. What are the reciprocal lattice vectors $\vec{b}_i$? What is the first Brillouin zone? Draw the free electron energy bands $E(\vec{k}+\vec{G}) = \hbar^2|\vec{k}+\vec{G}|^2/2m$ folded back into the first Brillouin zone. For simplicity, set $(k_x, k_y, k_z) = (k, 0, 0)$ so that you are just plotting E as a function of a single variable k. Do at least the first seven smallest $\vec{G}$ (lowest energies).

[**2.**] Consider electrons hopping in one dimension with a dispersion relation $E(k) = -2t\cos k$. Compute the density of states. Connect any features you notice in $E(k)$ to the plot of $E(k)$ versus k.

[**3.**] Sketch the density of states for the dispersion relation $E(k_x, k_y) = -2t\,[\cos k_x + \cos k_y]$. What lattice gives this $E(k_x, k_y)$? What physical system (class of materials) do solid state physicists hope to describe with this $E(k_x, k_y)$? Why might it be a reasonable choice (that is, what characteristic of this class of materials makes one want to use this dispersion relation?) What does the Fermi surface look like for Fermi energy near the bottom of the band (E just a bit more than $-4t$)? What does the Fermi surface look like for $E = 0$?

[**4.**] Consider the second quantized Hamiltonian

$$\hat{H} = -t \sum_l (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l) + \Delta \sum_l (-1)^l c_l^\dagger c_l$$

Write the matrix for $\hat{H}$ for one electron on an eight site lattice. That is, choose the occupation number basis $|1000\cdots0\rangle$, $|0100\cdots0\rangle$, $|0010\cdots0\rangle$, $\cdots$ and act with $\hat{H}$ on each state, writing the result as a matrix. Use periodic boundary conditions. What are the eight eigenvalues for $\Delta = 0$? What are the eight eigenvalues for $t = 0$? What are the eight eigenvalues for general t, Δ? (This last question is not so easy.)

[**5.**] Solve for the eigenenergies and eigenfunctions of the Schroedinger equation for a one dimensional delta function potential $V(x) = +g\,\delta(x)$.

[**6.**] State and prove Bloch's Theorem.

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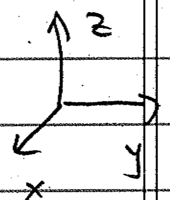
SOLUTIONS

Reciprocal lattice vectors:

$$\vec{b}_1 = \frac{2\pi}{\underbrace{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}_{V_c}}(\vec{a}_2\times\vec{a}_3) \quad \text{etc}$$

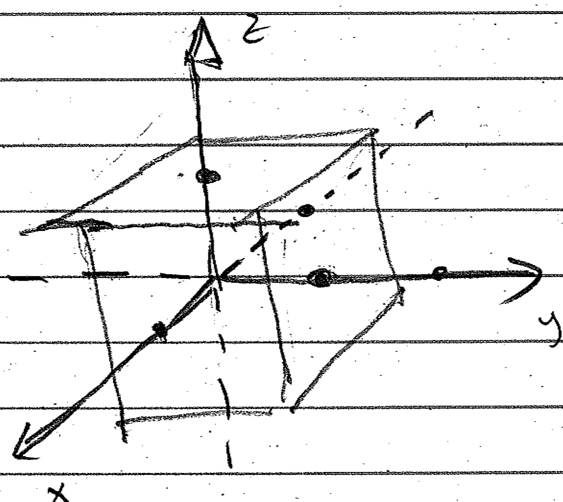


Here $\vec{a}_2\times\vec{a}_3 = a^2\,\hat{y}\times\hat{z} = a^2\hat{x}$

$$\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = a^3$$

So $\vec{b}_1 = \frac{2\pi}{a}\hat{x}$ likewise $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$ $b_3 = \frac{2\pi}{a}\hat{z}$

First BZ is formed by planes bisecting the reciprocal lattice vectors $\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$



cube centered at 0 and extending to $\pm a/2$ along each axis

1-2

For $\vec{G} = 0$ $\quad E(kkk) = \frac{\hbar^2}{2m} 3k^2 \leftarrow \frac{\hbar^2}{2m}\frac{3\pi^2}{a^2}$

at BZ bdy

$k = \pm \pi/a$

For $\vec{G} = \frac{2\pi}{a}\hat{x}$ or $\frac{2\pi}{a}\hat{y}$ or $\frac{2\pi}{a}\hat{z}$

$$E(\vec{k}+\vec{G}) = \frac{\hbar^2}{2m}\left[\left(k+\frac{2\pi}{a}\right)^2 + k^2 + k^2\right]$$

$$= \frac{\hbar^2}{2m}\left[3k^2 + \frac{4\pi k}{a} + \frac{4\pi^2}{a^2}\right]$$

Note that when $k = -\pi/a$ these match $\vec{G} = 0$ case

For $\vec{G} = -\frac{2\pi}{a}\hat{x}$ or $-\frac{2\pi}{a}\hat{y}$ or $-\frac{2\pi}{a}\hat{z}$

$$E(\vec{k}+\vec{G}) = \frac{\hbar^2}{2m}\left[3k^2 - \frac{4\pi k}{a} + \frac{4\pi^2}{a^2}\right]$$

These 3 match $\vec{G}=0$ at $k = {}^{+}\pi/a$

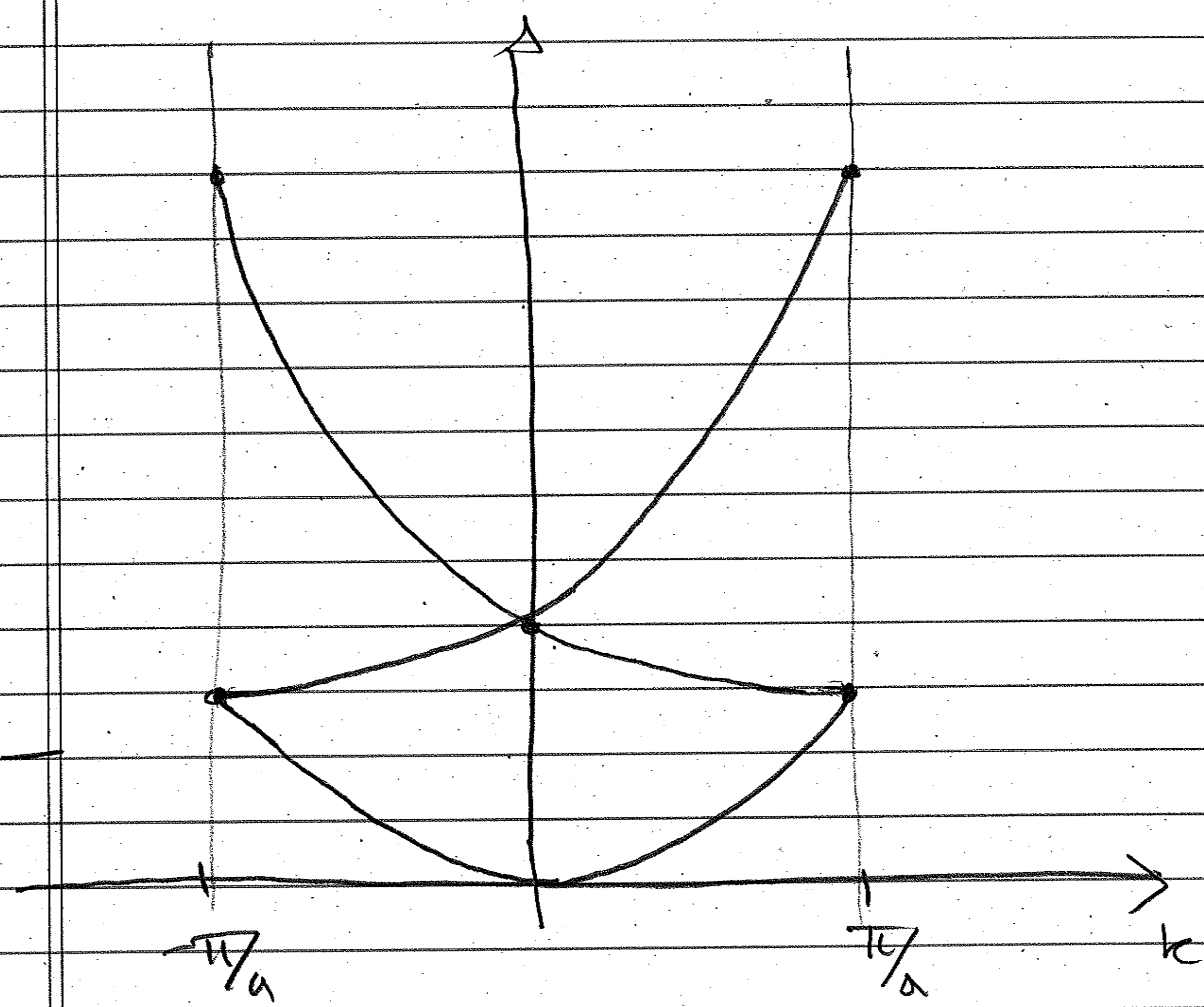
At $k=0$ the $\vec{G} = \pm\frac{2\pi}{a}\hat{x}, \pm\frac{2\pi}{a}\hat{y}, \pm\frac{2\pi}{a}\hat{z}$

all have $E = \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}$

They extend up to a maximum of

$$\frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\left\{3+4+4\right\} = \frac{\hbar^2}{2m}\frac{11\pi^2}{a^2}$$

So for these $\not{3}$ smallest $\vec{G}$ we get this picture:



2-1

$\boxed{2}$ $E(k) = -2t\cos k$

$$N(E) = \int \delta(E - E(k))\, dk$$

$$= \int \delta(E + 2t\cos k)\, dk$$

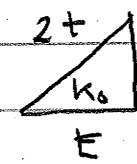
$$\delta(f(k)) = \frac{1}{|f'(k_0)|}\delta(k - k_0)$$ where k_0 is defined by $f(k_0) = 0$

$$f(k) = E + 2t\cos k$$

$$f'(k) = -2t\sin k$$

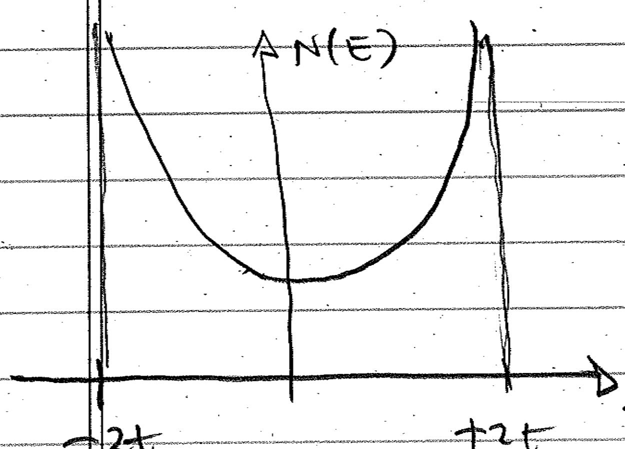
$$f(k_0) = E + 2t\cos k_0 = 0$$

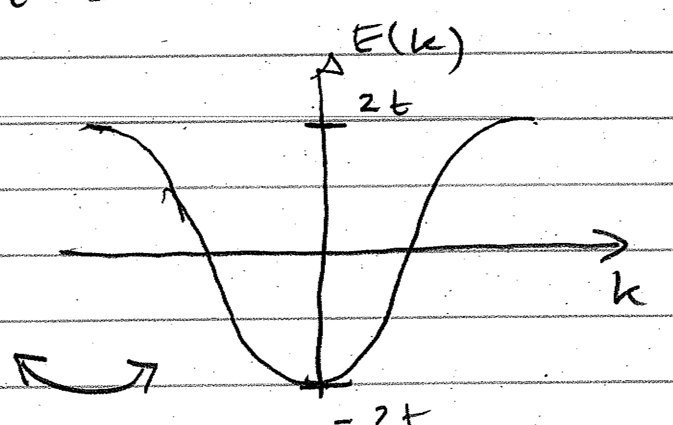
$$\cos k_0 = -E/2t$$



$$|f'(k_0)| = 2t\sin k_0 = 2t\,\frac{\sqrt{4t^2 - E^2}}{2t} = \sqrt{4t^2 - E^2}$$

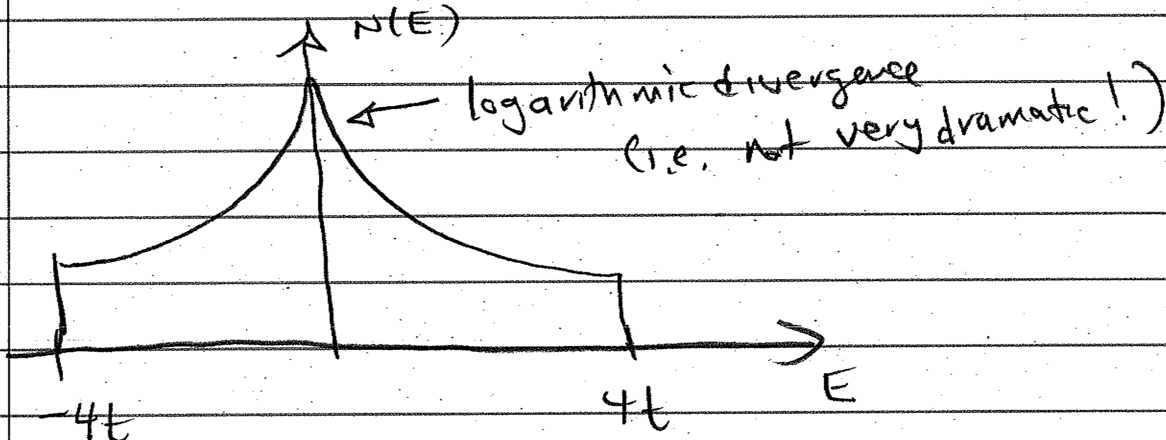
$$\therefore \quad N(E) = 1/\sqrt{4t^2 - E^2}$$





N(E) is big where E(k) is flat

We need to remember this famous $E(k_x, k_y)$ and its dispersion rel. It comes from a 2D square lattice tight binding Hamiltonian and



This $E(k)$ is used to describe high temperature superconductors, the Cu atoms in the CuO_2 planes form a square lattice, and it turns out holes do not sit on O atoms much so they can be (approximately) ignored

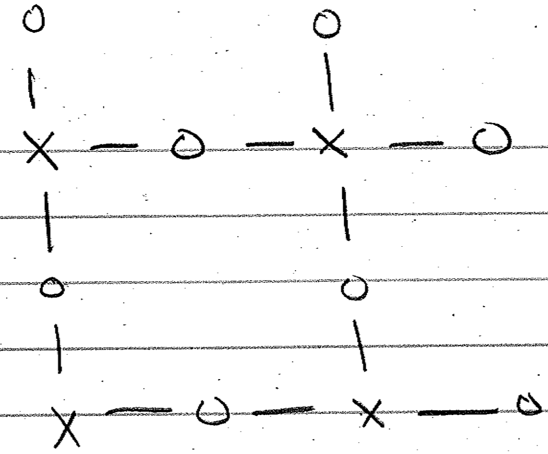
$La_{2-x}Sr_xCuO_4$
$Y_1Ba_2Cu_3O_{7+\delta}$
⋮
all have CuO_2 planes

3-2

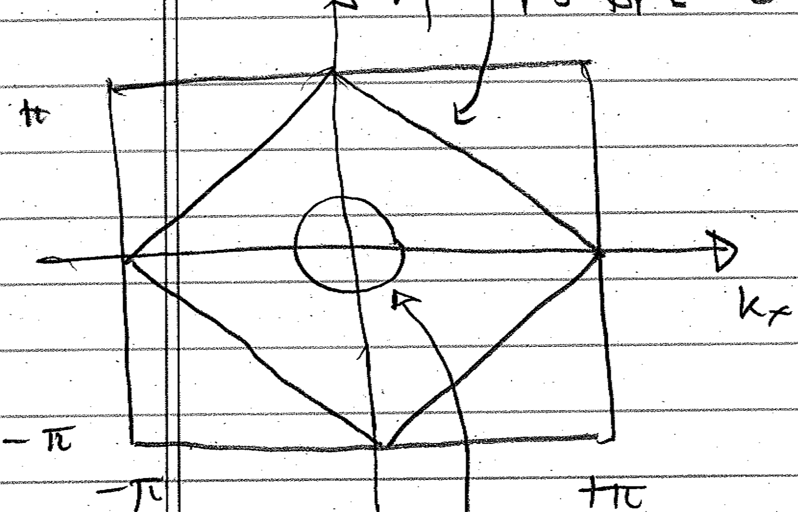
3 cont'd

X = copper

O = oxygen



FS for E = 0 (rotated square)



Δ ~ Again this is to be remembered from HW.

FS for $E \gtrsim -4t$

(circular)

$\hat{H}|10000000\rangle = -\Delta|10000000\rangle - t|01000000\rangle - t|00000001\rangle$

$\hat{H}|01000000\rangle = +\Delta|01000000\rangle - t|10000000\rangle - t|00100000\rangle$

$\vdots$

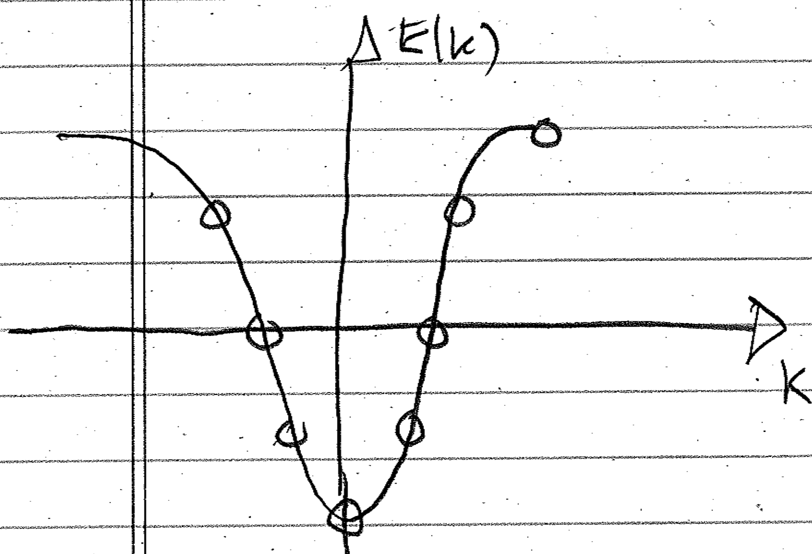
etc $\Rightarrow$

$$H = \begin{bmatrix} -\Delta & -t & 0 & 0 & & -t \\ -t & +\Delta & -t & 0 & & \\ 0 & -t & -\Delta & -t & & \\ 0 & 0 & 0 & \ddots & & \\ & & & & \ddots & \\ -t & & & & & \end{bmatrix}$$

tridiagonal (with pbc)

For $\Delta = 0$ Eigenvalues are $-2t\cos k$

with $k = \frac{2\pi}{8}\{-3, -2, -1, 0, 1, 2, 3, 4\}$



for $t=0$ matrix is diagonal, eigenvalues are
$+\Delta$ ← 4 fold
$-\Delta$ ← degenerate

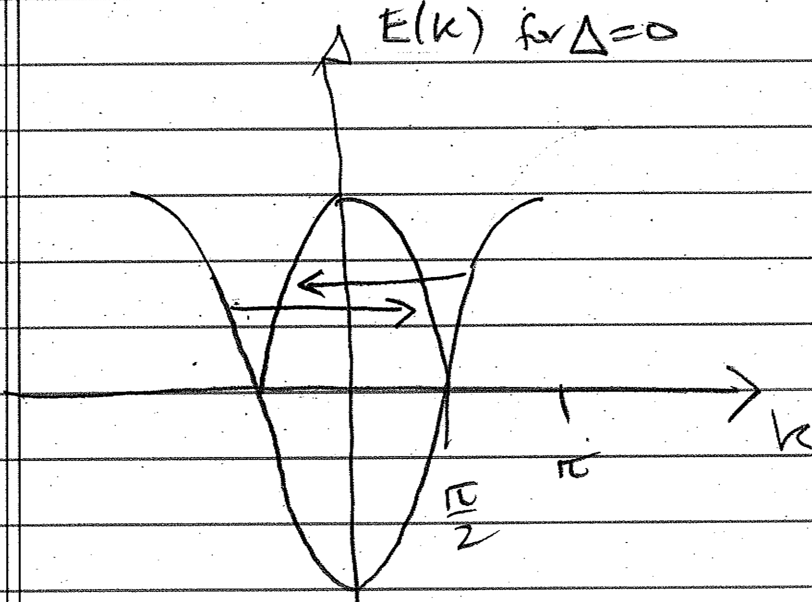
We discussed $\Delta \neq 0$, $t \neq 0$ case in class

The eigenvalues are

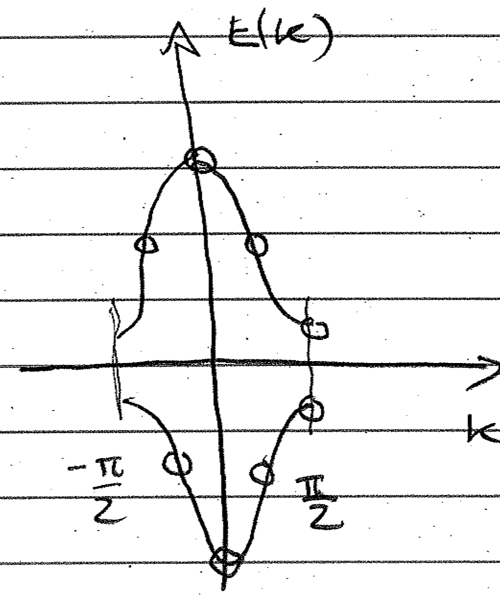
$$E(k) = \pm\sqrt{(-2t\cos k)^2 + \Delta^2}$$

where k values are now restricted to $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$

A picture:



First "fold in" to $-\frac{\pi}{2}, \frac{\pi}{2}$



then gap opens at BZ bdys

$\boxed{5}$ $$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - g\,\delta(x)$$

will have a bound state sol'n. Let's review that first, just for fun!

$$x \neq 0 \qquad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\text{so} \qquad H\psi = E\psi \implies \psi(x) = Ae^{\lambda x} + e^{-\lambda x}$$

$$E = -|E|$$

$$\frac{\hbar^2}{2m}\lambda^2 = |E|$$

Clearly $A = 0$ for $x > 0$
$B = 0$ for $x < 0$

Also look for symmetric solns $\psi(x) = \psi(-x)$

$$\psi(x) = \begin{cases} Ae^{\lambda x} & x < 0 \\ Ae^{-\lambda x} & x > 0 \end{cases}$$

Integrating Schroedinger Eqn through $x = 0$

$$\int_{-\epsilon}^{\epsilon}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - g\delta(x)\psi(x)\right]dx = -|E|\int_{-\epsilon}^{\epsilon}\psi(x)\,dx$$

$$\frac{\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{-\epsilon} - \left.\frac{d\psi}{dx}\right|_{+\epsilon}\right) - g\psi(0)$$

vanishes as $\epsilon \to 0$ since ψ bdd

5 cont'd

$$+\frac{\hbar^2}{2m}\left(\lambda A - (-\lambda A)\right) - gA = 0$$

$$A\left(\frac{\hbar^2\lambda}{m} - g\right) = 0$$

If $A \neq 0$ we conclude $\lambda = mg/\hbar^2$

and the bound state Energy is

$$-\left|\frac{\hbar^2\lambda^2}{2m}\right| = -\frac{\hbar^2}{2m}\frac{m^2g^2}{\hbar^4} = -\frac{mg^2}{2\hbar^2}$$

(A determined by normalization)

For $+g\delta(x)$ there are no bound state sol'ns ($E<0$)

$H\psi = E\psi \qquad \psi(x) = Ae^{ikx} + Be^{-ikx}$

$E>0 \qquad \hbar^2k^2/2m = E$

We can look for sol'ns arriving from left

$\psi(x) = e^{ikx} + re^{-ikx} \qquad x<0$

$te^{ikx} \qquad x>0$

Incident

reflected

transmitted

5 cont'd Continuity of ψ at $x=0$ requires

$$1+r=t$$

Doing same integral of Sch Eqn through $x=0$ as in -g case:

$$\frac{\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{-\epsilon}-\left.\frac{d\psi}{dx}\right|_{\epsilon}\right)+g\psi(0)=0$$

$$\frac{\hbar^2}{2m}\left[ik-ikr-ikt\right]+gt=0$$

Multiply by $\frac{mi}{\hbar^2 k}$ and define $\beta = {}^{mg}/_{\hbar^2 k}$

$$-\tfrac{1}{2}+\tfrac{r}{2}+\tfrac{t}{2}+i\beta t=0$$

using $r=t-1$

$$-\tfrac{1}{2}+\tfrac{t}{2}-\tfrac{1}{2}+\tfrac{t}{2}-i\beta t=0$$

$$t-1-i\beta t=0 \qquad t={}^{1}/_{1-i\beta}$$

then $r=t-1={}^{1}/_{1-i\beta}-1=\frac{1}{1-i\beta}(1-1+i\beta)$

$$r={}^{i\beta}/_{1-i\beta}$$

Blochs theorem states that the eigenstates of

$$\hat{H} = \frac{-\hbar^2 \nabla^2}{2m} + U(r)$$

with a periodic potential $U(r) = U(r+R)$

all R in Bravais lattice

can be written as

$$\psi_{nk}(r) = e^{ik \cdot r} u_{nk}(r)$$

plane wave
(soln with $U=0$!)

$u_{nk}(r) = u_{nk}(r+R)$

notice ψ itself does not have same periodicity as U.

Alternate statement $\psi(r+R) = e^{ik\cdot R}\psi(r)$

ie for any soln of $H\psi = E\psi$ there is a k such that

There are various possible proofs. The one we went through in class noted that $\hat{H}$ commutes with a whole set of translation operators.

Define

$$T_R f(r) \equiv f(r+R)$$

and $T_R T_{R'} = T_{R'} T_R$

And note $HT_R = T_R H$ because $U(r) = U(r+R)$

So, according to general principles of QM can look for sol'ns of $H\psi = E\psi$ by also asking $T_R\psi = \lambda\psi$

(This is how we solved Hydrogen atom: Found operators L^2 and L_z which commuted with H and then search for eigenfunctions of $\hat{H}$ from amongst those of L^2 and L_z)

Not only do $T_R, T_{R'}$ commute but eigenvalues obey

$$T_R\psi = c(R)\psi$$

$$T_{R'}\psi = c(R')\psi$$

$$T_{R+R'}\psi = c(R+R')\psi \qquad c(R+R') = c(R)c(R')$$

Thus if we define $c(a_i) = e^{2\pi i x_i}$

primitive lattice vectors

6-3

we have for $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$$c(\vec{R}) = e^{2\pi i(n_1 x_1 + n_2 x_2 + n_3 x_3)}$$

Defining $\vec{k} = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3$

reciprocal lattice vectors

and using $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$

we see $c(\vec{R}) = e^{i\vec{k}\cdot\vec{R}}$

Thus $\psi(r+R) = T_R\psi(r) = c(R)\psi(r)$

$$= e^{i\vec{k}\cdot\vec{R}}\psi(r)$$