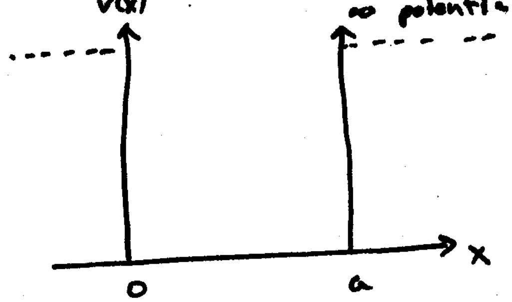
1.a)



$$\vec{\nabla}^2\psi(x) + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) = 0$$

and $V(x) = 0$ for $0 < x < a$ $\qquad \nabla = \frac{\partial^2}{\partial x^2}$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) = 0$$

$\psi(x) = A_1 \cos kx + A_2 \sin kx$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$

and $k = \frac{2\pi}{\lambda} = \frac{n\pi}{a}$

Using Boundry Conditions:

$$\psi(x=0) = 0 = A_1 \cos k(0) + A_2 \overset{0}{\cancel{\sin k(0)}} \implies A_1 = 0$$

$$\psi(x=a) = 0 = \overset{0}{\cancel{A_1}} \cos(0) + A_2 \sin ka$$

$k = \frac{n\pi}{a}$ because $\sin = 0$ at multiples of π

use $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

$$\int_0^a A_2^2 \sin^2 kx \, dx = 1$$

$$A_2 = \sqrt{\frac{2}{a}}$$

so $\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ for $n = 1, 2, 3, \ldots$

1.a) Expected Value

$$\langle x \rangle = \int_0^a \psi^*(x)\,\psi(x)\,x\,dx$$

$$= \int_0^a \sqrt{\tfrac{2}{a}}\,\sin\left(\tfrac{n\pi x}{a}\right)\cdot\sqrt{\tfrac{2}{a}}\,\sin\left(\tfrac{n\pi x}{a}\right) x\,dx$$

$$= \frac{2}{a}\int_0^a x\sin^2\left(\tfrac{n\pi x}{a}\right)dx \Rightarrow \text{use} \quad \sin^2 x = 1-\cos 2x$$

$$= \frac{2}{a}\int_0^a \frac{x}{2}\left(1-\cos\left(\tfrac{2n\pi x}{a}\right)\right)dx$$

$$= \frac{1}{a}\int_0^a x\,dx - \frac{1}{a}\int_0^a x\cos\left(\tfrac{2n\pi x}{a}\right)dx$$

$$= \frac{1}{2a}x^2\Big|_0^a - \frac{1}{a}\left(\frac{\cos()x}{a^2} + \frac{x\sin()x}{a}\right)\Big|_0^a$$

$$= \frac{a}{2} - \left[\frac{\cos\left(\frac{2n\pi a}{a}\right)}{a^3} + \frac{a\overbrace{\cancel{\sin\left(\frac{2n\pi a}{a}\right)}}^{0}}{a^2} - \frac{\cos\left(\frac{2n\pi(0)}{a}\right)}{a^3} - \frac{\overbrace{\cancel{0\sin}}^{0}}{a^2}\right]$$

$$= \frac{a}{2} - \left[\frac{\overbrace{\cancel{\cos(2n\pi)}}^{1 \text{ for all } n}}{a^3} - \frac{\overbrace{\cancel{\cos(0)}}^{1}}{a^3}\right] \qquad n = 1, 2, 3, \ldots$$

$$\langle x \rangle = \frac{a}{2} \qquad \text{(for all three energy levels)}$$

This makes sense as we would expect that the average position of the electron would balance out in the center of the well.

1a)

$$\langle \vec{p} \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{j} \vec{\nabla} \psi \, dx$$

$$= \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \frac{\hbar}{j} \frac{\partial}{\partial x} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{2}{a} \frac{\hbar}{j} \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) \frac{\partial}{\partial x} dx$$

$$= \frac{2}{a} \frac{\hbar}{j} \int_0^a 2 \sin\left(\frac{n\pi x}{a}\right) \left(\frac{n\pi}{a} \cos \frac{n\pi x}{a}\right) dx \quad 0$$

$\langle \vec{p} \rangle = 0$ for all n

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n^2 \pi^2}{a^2}\right)$$

$m = m_o = 9.11 \times 10^{-31}$ kg ; $\hbar = 1.054 \times 10^{-34}$ J-s

$$E_n = \frac{6.02 \times 10^{-38} \, n^2}{a^2} \cancel{J\text{-}s} \left(\frac{1 \, eV}{1.6 \times 10^{-19} \cancel{J\text{-}s}}\right) = 3.76 \times 10^{-19} \frac{n^2}{a^2} \, eV$$

$$E_1 = \frac{3.76 \times 10^{-19}}{a^2} \, eV \quad ; \quad E_2 = \frac{1.5 \times 10^{-18}}{a^2} \, eV \quad ; \quad E_3 = \frac{3.38 \times 10^{-18}}{a^2} \, eV$$

The expected value for momentum also is acceptable at zero for a stable system. The Increasing energy corresponds to the increasing frequency supported

1.b) Check the Heisenberg uncertainty principle

$$\Delta x \Delta p_x \geq \hbar$$

where $\langle \Delta x \rangle = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ we have $\langle x \rangle$ so we need

$\boxed{n=1}$

$$\langle x^2 \rangle = \int_0^a \sqrt{\tfrac{2}{a}} \sin\left(\tfrac{\pi x}{a}\right) x^2 \sqrt{\tfrac{2}{a}} \sin\left(\tfrac{\pi x}{a}\right) dx = \tfrac{2}{a}\int_0^a x^2 \sin^2\left(\tfrac{\pi x}{a}\right) dx$$

$\boxed{k=\frac{\pi}{a}}$

$$= \frac{2}{a}\int_0^a x^2 \left(1 - \tfrac{1}{2}\cos 2kx\right) dx = \frac{1}{a}\left[\frac{x^3}{3} - \frac{2x\cos 2kx}{4k^2} - \frac{4k^2x^2 - 2}{8k^3}\sin 2kx\right]_0^a$$

$$= \frac{1}{a}\left[\frac{x^3}{3} - \frac{xa^2}{2\pi^2}\cos\left(\cancel{\tfrac{2\pi}{a}x}\right)^{1} - (\quad)\sin\left(\cancel{\tfrac{2\pi}{a}x}\right)^{0}\right]_0^a$$

$$= \frac{1}{a}\left(\frac{a^3}{3} - \frac{a^3}{2\pi^2} - 0\right) = \frac{a^2}{3} - \frac{a^2}{2\pi^2}$$

$$\langle \Delta x \rangle = \sqrt{\frac{a^2}{3} - \frac{a^2}{2\pi^2} - \left(\frac{a}{2}\right)^2} = a\sqrt{\frac{1}{3} - \frac{1}{2\pi^2} - \frac{1}{4}}$$

So what uncertainty is smaller, position with a small atomic spacing (a) or the momentum that follows:

$$\langle p_x^2 \rangle = \int_0^a \sqrt{\tfrac{2}{a}} \sin\left(\tfrac{\pi x}{a}\right)\left(-\hbar^2\frac{\partial}{\partial x}\right)\sqrt{\tfrac{2}{a}} \sin\left(\tfrac{n\pi}{a}\right) dx$$

$$= \frac{2\pi^2\hbar^2}{a^3}\int_0^a \sin^2\left(\tfrac{\pi x}{a}\right) dx = \frac{\pi^2\hbar^2}{a^2}$$

$$\langle \Delta p_x \rangle = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \frac{\pi\hbar}{a}$$

$$\langle \Delta x \rangle \langle \Delta p \rangle = \pi\hbar\sqrt{\frac{1}{3} - \frac{1}{2\pi^2} - \frac{1}{4}} \geq \frac{\hbar}{2}$$ (use $\hbar/2$ for standard deviation)

$$0.57 \geq \frac{1}{2}$$

So the uncertainty principle holds

4/

2. $E = A(2k_x^2 + k_y^2) - B(k_x^4 + 3k_y^4)$

(a) Find wavevector k w/ $v = 0$

from eq (27) on Review of QM

$$v_g = \frac{1}{\hbar} \vec{\nabla}_k E$$

where $\nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ operator :

$$\therefore \vec{v}_g = \frac{1}{\hbar}\left(4k_x A - 4k_x^3 B\right)\hat{x} + \frac{1}{\hbar}\left(2Ak_y - 12Bk_y^3\right)\hat{y} = 0$$

$$\boxed{k_x = 0, \pm\sqrt{\frac{A}{B}}} \quad \text{\&} \quad \boxed{k_y = 0 \pm \sqrt{\frac{A}{6B}}}$$

$$2Ak_y - 12Bk_y^3 = 0$$

$$6Bk_y^2 = A\cancel{k_y}$$

$$k_y = \sqrt{\frac{A}{6B}}$$

$$\vec{k} = k_x\hat{x} + k_y\hat{y}$$

For energies substitute in $E = A(\ ) - B(\ )$ from above

for $(k_x, k_y) = (0, 0)$ $\qquad E = 0$

$(k_x, k_y) = \left(0, \pm\sqrt{\frac{A}{6B}}\right)$ $\qquad E = A\left(\frac{A}{6B}\right) - B\left(3\frac{A^2}{6^2B^2}\right) = \frac{A^2}{11B}$

$(k_x, k_y) = \left(\pm\sqrt{\frac{A}{B}}, 0\right)$ $\qquad E = A\left(\frac{2A}{B}\right) - B\left(\frac{A^2}{B^2}\right) = \frac{A^2}{B}$

$(k_x, k_y) = \left(\pm\sqrt{\frac{A}{B}}, \pm\sqrt{\frac{A}{6B}}\right)$ $\qquad E = \frac{5A^2}{4B}$

2. (cont.)

To determine whether points are max or min look at 2^{nd} derivative of E:

$$\frac{\partial^2 E}{\partial k_x^2} = 4A - 12B k_x^2$$

$$\frac{\partial^2 E}{\partial k_y^2} = 2A - 36Bk_y^2$$

$$\frac{\partial^2 E}{\partial k_x \partial k_y} = 0$$

To test for max and min use

if: $\frac{\partial^2 f}{\partial x^2} - \left(\frac{\partial f}{\partial x \partial y}\right)^2 > 0$ & $\frac{\partial^2 f}{\partial x^2} > 0 \Rightarrow$ minima

" > 0 & " $< 0 \Rightarrow$ maxima

" $< 0 \Rightarrow$ saddle point

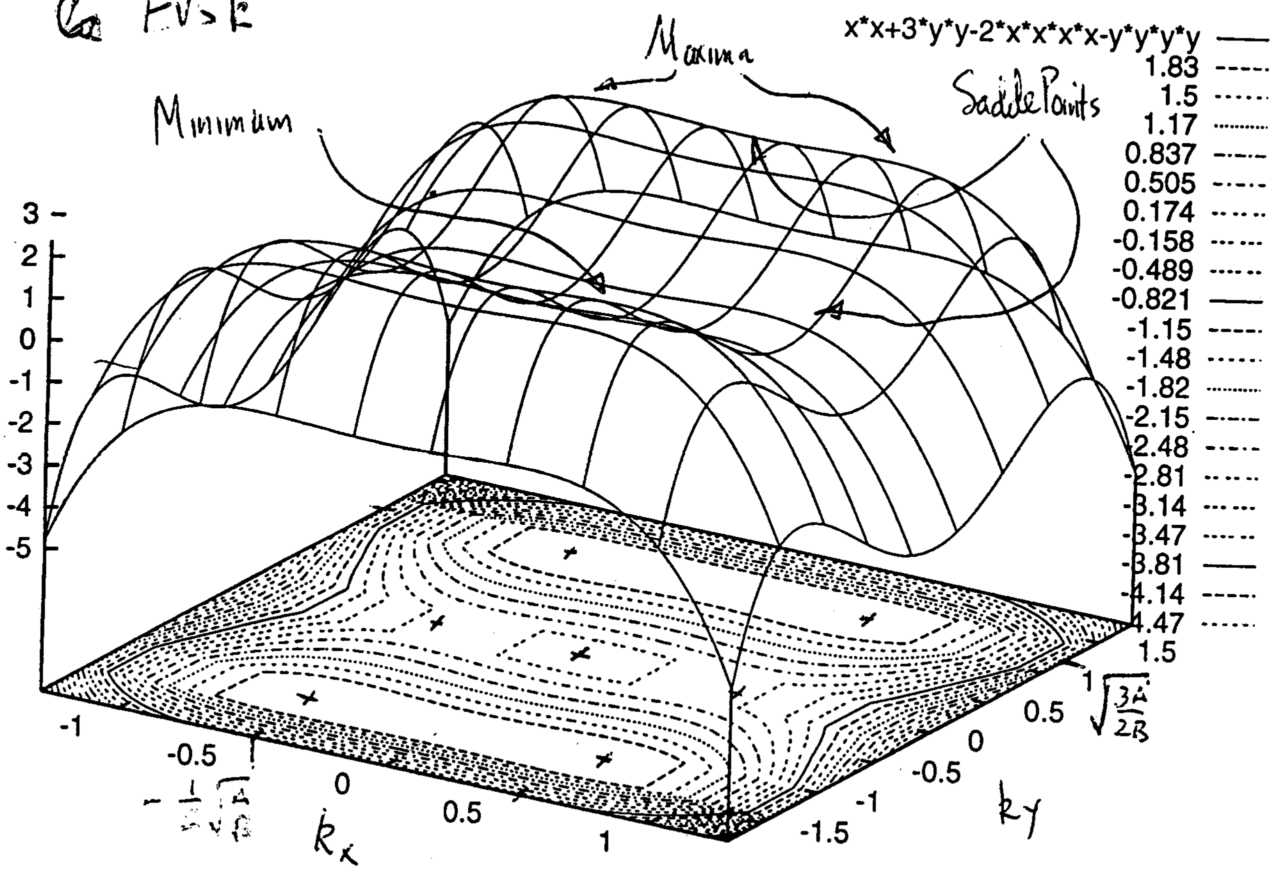
$\left(\pm\sqrt{\frac{A}{B}}, \pm\sqrt{\frac{A}{6B}}\right)$ is a maxima

$\left(0, \pm\sqrt{\frac{A}{6B}}\right)$ and $\left(\pm\sqrt{\frac{A}{B}}, 0\right)$ are saddle points

This can be plotted and solved it MATLAB or Maple.

Note: Use appropriate $\frac{\partial E}{\partial k_x}$ terms

(a) E vs k



(b)

$$M^{-1} = \frac{1}{\hbar^2}\begin{bmatrix} \frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} \\ \frac{\partial^2 E}{\partial k_y k_x} & \frac{\partial^2 E}{\partial k_y^2} \end{bmatrix} = \frac{1}{\hbar^2}\begin{bmatrix} 2A - 24Bk_x^2 & 0 \\ 0 & 6A - 12Bk_y^2 \end{bmatrix}$$

$= \frac{1}{\hbar^2}\begin{bmatrix} 2A & 0 \\ 0 & 6A \end{bmatrix}$ at $(0,0)$ $\Rightarrow$ e^--like (positive m^*)

$= \frac{1}{\hbar^2}\begin{bmatrix} -4A & 0 \\ 0 & -12A \end{bmatrix}$ at $\left(\pm\frac{1}{2}\sqrt{\frac{A}{B}}, \pm\sqrt{\frac{3A}{2B}}\right) \Rightarrow h^+$-like

$$\left.\begin{aligned} &= \frac{1}{\hbar^2}\begin{bmatrix} 2A & 0 \\ 0 & -12A \end{bmatrix} \text{ at } \left(0, \pm\sqrt{\tfrac{3A}{2B}}\right) \\ &= \frac{1}{\hbar^2}\begin{bmatrix} -4A & 0 \\ 0 & 6A \end{bmatrix} \text{ at } \left(\pm\tfrac{1}{2}\sqrt{\tfrac{A}{B}}, 0\right) \end{aligned}\right\}$$ neither h^+ nor e^--like (saddle points)

(c) $\vec{F} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $\vec{x} = (0, 0)$

$$\vec{a} = M^{-1}\vec{F} = \begin{pmatrix} 2A & 0 \\ 0 & 6A \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2A \\ 6A \end{pmatrix}$$

or $\begin{pmatrix} 1 \\ 3 \end{pmatrix}$ direction

(d) $\vec{F} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $\vec{x} = \left(\frac{1}{2}\sqrt{\frac{A}{B}}, \sqrt{\frac{3A}{2B}}\right)$

$$\vec{a} = \begin{pmatrix} -4A & 0 \\ 0 & -12A \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -4A \\ -12A \end{pmatrix}$$

or $-\begin{pmatrix} 1 \\ 3 \end{pmatrix}$ direction

3. The outer energy band of a crystal of N atoms per unit vol. is described

by $E = E_0 + \frac{\hbar^2 (k-k_0)^2}{2m_e^*}$. & the band contains one e^- per atom.

(a) Is this material an insulator, a metal or a semiconductor?

If the crystal has N atoms per unit vol., the outermost band can at most have 2N states, i.e. 2 electrons per atom (spin up & down); now this band has one e^- per atom $\Rightarrow$ partially full. A material that has its outermost band partially full is a $\boxed{\text{metal}}$.

(b) What would $E_f - E_0$ be at $0°K$ in terms of m_e^*?

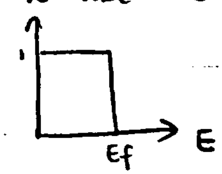
This outermost band of the metal is similar to the conduction band in semiconductors described by Eq. (24), with $k_c \to k_0$, $E_c \to E_0$

$\therefore$ from equation (36) carrier conc. $n = \int_{E_0}^{\infty} f_{FD}(E) N_c(E) dE$ — ①

→ Here, the carrier conc. $n = N$

→ We're at $0°K$, $\therefore$ we have to use the exact fermi-dirac distribution.

At 0K, $f_{FD}(E)$ looks like:



i.e. $f_{FD}(E) = 1$ for $E < E_f$

$= 0$ for $E > E_f$

$\therefore$ in the above integral, we can let the upper limit of integration be E_f, and let $f_{FD}(E) = 1$

→ From (29) $N_c(E) = \frac{4\pi}{h^3}(2m_e^*)^{3/2}(E-E_0)^{\frac{1}{2}} dE$

Substitute these data into ①:

$$N = \int_{E_0}^{E_f} \frac{4\pi}{h^3}(2m_e)^{\frac{3}{2}}(E-E_0)^{\frac{1}{2}} dE$$

Let $E' = E - E_0$ $\therefore dE' = dE$ & the limits of integration is from $E' = 0$ to $E_f - E_0$

$$\therefore N = \int_0^{E_f - E_0} \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}} E'^{\frac{1}{2}} dE'$$

$$= \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}} \left(\frac{2}{3}E'^{\frac{3}{2}}\right)\Big|_0^{E_f - E_0}$$

$$= \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}}\left(\frac{2}{3}(E_f - E_0)^{\frac{3}{2}}\right)$$

$$\therefore (E_f - E_0)^{\frac{3}{2}} = \frac{3}{8}\frac{h^3}{\pi}\frac{N}{(2m_e^*)^{\frac{3}{2}}}$$

$$\Rightarrow (E_f - E_0) = \boxed{\left(\frac{3N}{8\pi}\right)^{\frac{2}{3}} \frac{h^2}{2m_e^*}}$$

4. Above E_F : $f_{M-B} = \exp\left[-\frac{E-E_F}{k_BT}\right]$

for $\left|\frac{f_{M-B}}{f_{F-D}} - 1\right| < 0.03$

$$\exp\left(-\frac{E-E_F}{kT}\right)\left(1+\exp\left(\frac{E-E_F}{kT}\right)\right) - 1 < 0.03$$

$$\exp\left(-\frac{E-E_F}{kT}\right) < 0.03$$

$$E > E_F - kT \ln(0.03)$$

$$> E_F + 0.0913\,eV$$

Below E_F : $f_{M-B} = 1 - \exp\left(\frac{E-E_F}{kT}\right)$

for $\left|\frac{f_{M-B}}{f_{F-D}} - 1\right| < 0.03$,

$$\left(1-\exp\left(\frac{E-E_F}{kT}\right)\right)\left(1+\exp\left(\frac{E-E_F}{kT}\right)\right) - 1 > -0.03$$

$$\exp\left(\frac{2(E-E_F)}{kT}\right) < 0.03$$

$$E < E_F + \frac{kT}{2}\ln(0.03)$$

$$E < E_F - 0.046\,eV$$

4.
cont.