Problem 1 (25 pts)
Find the electron energy and wavefunction in a one-dimensional quantum well:

\[ V(x) = \begin{cases} 
+ \infty, & \text{when } 0 > x \text{ or } x > 3L \\
0, & \text{when } 0 < x < 3L 
\end{cases} \]
Infinite - Barrier Quantum well

at $0 < x < 3L$ Schrödinger Eq. $1 - D$

$$-\frac{k^2}{2m} \frac{d^2 \Psi}{dx^2} \Psi = E \Psi \quad \text{(I)}$$

Let $k^2 = \frac{2mE}{\hbar^2}$. (I) becomes $\frac{d^2 \Psi}{dx^2} \Psi + k^2 \Psi = 0$

$\therefore \Psi = A \sin kx + B \cos kx$

We Boundary Conditions $\Psi(0) = \Psi(3L) = 0$

$\Rightarrow B = 0$, $k = \frac{n\pi}{3L}$, $n = \pm 1, \pm 2, \ldots$

We $\int_0^\infty |\Psi|^2 dx = 1 \Rightarrow A = \sqrt{\frac{2}{3L}}$

$\therefore \Psi(x) = \sqrt{\frac{2}{3L}} \sin \frac{n\pi x}{3L}$, $E_n = \frac{n^2\hbar^2 \pi^2}{18mL^2}$ (at $0 < x < 3L$)

at $x < 0$ or $x > 3L$ $\Psi(x) = 0$
Problem 2 (MOS structure and confined state) (25 pts)

(1) As shown in Fig. 1, a MOS structure on a shallow np junction can be simply considered as a quantum well. Please find the electron confined state energy $E$ ($E < V_0$, $V_0$ is about 1 eV). You can just list the equation to calculate $E$. The equation include only $E$, $V_0$, and $a$.

(2) Please draw the first confined state wavefunction vs position $y$. 
P2. \( V_{00} = \infty \quad x < 0 \quad \text{Region 1} \)
\( = V_0 \quad 0 < x < a \quad \text{Region 2} \)
\( = 0 \quad x > a \quad \text{Region 3} \)

For confined state \( E < V_0 \)

For Region 1: \( N_2(x) = 0 \)

For Region 2:
\[-\frac{k^2}{2m} \frac{d^2}{dx^2} N_2(x) = E N_2(x)\]
\[\Rightarrow N_2(x) = A \sin k x + B \cos k x\]

where \( k^2 = \frac{2mE}{k^2} \).

We B.C. \( N_2(0) = 0 \Rightarrow B = 0 \)

\[N_2(x) = A \sin k x\]

For Region 3:
\[-\frac{k^2}{2m} \frac{d^2}{dx^2} N_3(x) + V_0 N_3(x) = E N_3(x)\]
\[\Rightarrow \frac{d^2}{dx^2} N_3(x) = \frac{2m(V_0 - E)}{k^2} N_3(x)\]
\[\Rightarrow N_3(x) = C e^{k_1 x} + D e^{-k_1 x}\]

where \( k_1 = \frac{2m(V_0 - E)}{k^2} \).

We B.C. \( N_3(0) = 0 \Rightarrow C = 0 \)

\[N_3(x) = D e^{-k_1 x}\]
Problem 3 (25 pts)

(1) For an electron in the \((n, l, m) = (2, 1, 1)\) state of hydrogen, determine the expectation value of position.

(2) For \(n = 6\), what is the possible states of the electron in the hydrogen atom?

\[
\langle r \rangle \quad \text{(or use } \langle r^2 \rangle) \\
= \int_0^{2\pi} \int_0^{\pi} \int_0^\infty r^4 e^{-\frac{r}{a_0}} \sin \theta \, dr \, d\theta \, d\Phi \\
= (2\pi) \left( \int_0^{\pi} (\cos^2 \theta - 1) \, d\cos \theta \right) \int_0^\infty \left( \frac{1}{\sqrt{3}\sqrt{2\pi a_0^3}} \, e^{-\frac{r}{a_0}} \cdot \frac{1}{2\pi} \right)^2 \, dr \\
= 2\pi \cdot \left( \frac{4}{3} \right) \cdot \left( \frac{1}{64\pi a_0^4} \right) \left( + 120 a_0^5 \right) \\
= 5 a_0
\]
Problem 4 (25 pts)

(1) From the E-k relationship of graphene, prove band gap of graphene = 0?

(2) From the E-k relationship of graphene, please find all the \( k(k_x, k_y) \) points.

(3) Prove the electrons in graphene are Dirac Fermions. Find the E-k equations when \( k \) is very close to these \( k \) points (found in question (2)).

(4) What CNT \((n, m)\) if it is formed by wrapping the graphene from O to C or from O to T? what is the diameter for the CNT? Are they metallic or semiconducting? If it is semiconductor, what is the band gap? (see the following figure)
(1) You can prove it like the homework 5.21 by putting the six corner in k-space.

Or we can prove it by finding $\Delta E_g = 0$

$$\Delta E_g = E_+ - E_-$$

$$\sim 2\gamma_0 \sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$

To have zero “bandgap”, we should have $(k_x, k_y)$ to make $\Delta E_g = 0$.

$$1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right) = 0$$

So:

$$\cos\left(\frac{k_y a}{2}\right) = \frac{-4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \pm \sqrt{f(k_x)}}{8}$$

where $f(k_x) = 16 \cos^2\left(\frac{\sqrt{3}k_x a}{2}\right) - 16$

In order to have real solution for $k_y$, it must have

$$f(k_x) \geq 0$$

However,

$$\cos^2\left(\frac{\sqrt{3}k_x a}{2}\right) \leq 1$$
Therefore, \( \cos \left( \frac{\sqrt{3} k_x a}{2} \right) = \pm 1 \)

\( \Rightarrow k_x = 0; \text{ or } k_x = \pm \frac{2\pi}{\sqrt{3}a} \) (only within the FBZ)

Because: \( \cos \left( \frac{\sqrt{3} k_x a}{2} \right) = \pm 1 \)

When \( k_x = 0 \), \( \cos \left( \frac{k_y a}{2} \right) = -\frac{1}{2} \Rightarrow k_y = \pm \frac{4\pi}{3a} \)

When \( k_x = \frac{2\pi}{\sqrt{3}a} \), \( \cos \left( \frac{k_y a}{2} \right) = \frac{1}{2} \Rightarrow k_y = \pm \frac{2\pi}{3a} \)

When \( k_x = -\frac{2\pi}{\sqrt{3}a} \), \( \cos \left( \frac{k_y a}{2} \right) = \frac{1}{2} \Rightarrow k_y = \pm \frac{2\pi}{3a} \)

Therefore, there are totally 6 corners to have \( \Delta E_g = 0 \).

\( (0, \pm \frac{4\pi}{3a}) ; (\pm \frac{2\pi}{\sqrt{3}a}, \pm \frac{2\pi}{3a}) \)
Second method:

Find maximum or minimum point

\[ \frac{\delta E_k}{\delta k_x} = 0 \Rightarrow \sin \left( \frac{\sqrt{3}}{2} k_x a \right) \cos \left( \frac{\pi}{2} \right) = 0 \]

\[ \Rightarrow k_x = 0 \text{ or } k_x = \pm \frac{2\pi}{3a} \]

Max for \( E_- \)

Min for \( E_+ \)

or \( k_y = \pm \frac{\pi}{a} \)

Max for \( E_+ \)

Min for \( E_- \)

So we only \( k_x = 0, \pm \frac{2\pi}{3a} \)

\[ \frac{\delta E_k}{\delta k_y} = 0 \Rightarrow 2 \cos \frac{k_x a}{2} \sin \frac{k_x a}{2} + \cos \frac{\sqrt{3}}{2} k_x a \sin \frac{k_x a}{2} = 0 \]

Put \( k_x = 0, \pm \frac{2\pi}{3a} \) in to find \( k_y \)

\[ k_x = 0, k_y = \pm \frac{4\pi}{3a} \]

\[ k_x = \pm \frac{2\pi}{3a}, k_y = \pm \frac{2\pi}{3a} \]

Note \( k_x, k_y \) must in 1st 8 2nd.
(3) Prove the electrons in graphene are Dirac Fermions. Find the E-k equations when k is very close to these k points (found in question (2)).

Solve: in one dimension when \( k_x = 0 \)

Consider only \( k_y \) direction \( k_y \sim \frac{4\pi}{3a} \), E, \( E_k \) become

\[
\gamma_0 \sqrt{1 + 4 \cos \left( \frac{k_ya}{2} \right) + 4 \cos^2 \left( \frac{k_ya}{2} \right)}
\]

\[
= \gamma_0 \left( 1 + 2 \cos \left( \frac{k_ya}{2} \right) \right) \approx 0
\]

Therefore, we can expand it around \( k_y = \frac{4\pi}{3a} \)

\[
E_k \sim \pm \gamma_0 \left( a - \frac{2}{2} \sin \left( \frac{4\pi}{3a} \cdot \frac{a}{2} \right) \left( k_y - \frac{4\pi}{3a} \right) \right)
\]

\[
E_k \sim \pm \gamma_0 \frac{\sqrt{3}}{2} \left( k_y - \frac{4\pi}{3a} \right)
\]

Similarly, when \( k_y = \frac{4\pi}{3a} \), find E, \( E_k \) around \( k_x = 0 \)

\[
\pm \gamma_0 \sqrt{1 - 2 \cos \left( \frac{\sqrt{3}k_xa}{2} \right) + 4 \left( \frac{1}{4} \right)}
\]

\[
= \pm \gamma_0 2 \sin \left( \frac{\sqrt{3}k_xa}{4} \right)
\]
Therefore, we can expand it around $k_x=0$

$$E_k \sim \pm \gamma_0 \frac{\sqrt{3}}{2} k_x$$

The slopes along $k_x$ and $k_y$ are the same.

Similarly, we can find out that $E_k$ is linear with $k_x$ and $k_y$ around these $k$ points.

(4) What CNT (n, m) if it is formed by wrapping the graphene from O to C or from O to T? What is the diameter for the CNT? Are they metallic or semiconducting? If it is semiconductor, what is the band gap?

Solve:

From $O \rightarrow C$, the CNT is (4, 2) CNT

$$d = \frac{\sqrt{3}}{2\pi} b \sqrt{n^2 + nm + m^2} = \frac{\sqrt{3}}{2\pi} b \sqrt{28} = \frac{\sqrt{21}}{\pi} b$$

Since $(2n+m)/3=10/3$ is not an integer, it is a semiconducting CNT.

From $O \rightarrow T$, the CNT is (4, 1) CNT

$$d = \frac{3b}{2\pi} \sqrt{7}$$

Since $(2n+m)/3=3$, it is metallic.