Solution Q 1

1. A wave function is physically valid if it is square integrable, single-valued, continuous, and has continuous first derivatives. The given wave function is however, not continuous at L and $-L$. We can show this quite easily. Approaching $-L$ from the "left side" of the x axis, we see that the left hand limit is zero.

$$\lim_{x \to -L^-} \psi(x) = 0. \tag{1}$$

However, if we calculate the "right hand limit", we find

$$\lim_{x \to -L^+} \psi(x) = A\left(1 + \frac{1}{\sqrt{2}}\right) \neq 0. \tag{2}$$

Since the function is discontinuous, we can conclude that the wave function is not physically valid.

NOTE: Merely calculating the value of the function and its derivative at L or $-L$ will not be given any marks. You have to justify your answer and argue that it is discontinuous.

2. $A = \left(3L + \dfrac{8\sqrt{2}L}{\pi} + \dfrac{2L}{\pi}\right)^{-1/2}$.

The integration is extremely straightforward and you will be awarded full-marks if you get the above answer. If you have made a typographical error while writing down the answer, a certain amount of marks will be deducted based on the severity of the error. Furthermore, failure to get the correct answer, or doing the integration incorrectly will not earn you any marks.

You also have to show all the steps explicitly.

3. Since the wave function is not physically valid, it will not be an eigen function of the Hamiltonian operator. Hence it will not have an energy eigen value. Furthermore, the potential is not specified in the problem, so it is not possible to even calculate the eigen values explicitly. But you will be given marks, even if you show that this wave function is not an energy eigen function of the infinite square well. The point is, this was a conceptual question: we were not expecting you to do any calculations as such.

4. Since this wave function is not physically valid, it is unlikely to satisfy the uncertainty principle. You will be given full-marks, if you have written down this simple statement. You will receive partial marks (1.5), if you have written down all the formulas used for calculating $< x >, < x^2 >, < p >, < p^2 >$, and the expressions for $\Delta x, \Delta p$ and stated the uncertainty principle $(0.5 + 0.5 + 0.5)$. You will get one additional mark for showing explicitly that $< x >= 0$. You can do the integration explicitly or argue from the fact that the integrand is and even/odd function.

Solution 2.1

(a) The system possesses two degrees of freedom so that two generalized coordinates are required. For these we use θ_1, the angle of rotation of the lower cylinder, and θ, the angle made by the plane containing the two axes of the cylinders and the vertical.

Initially the plane containing the two axes of the cylinders is vertical. At a later time, this plane makes an angle θ with the vertical. The original point of contact, A, now moves to A' on the lower cylinder and to A'' on the upper cylinder. With the angles so defined we have from Fig. 2.4

$$\theta_1 + \theta = \theta_2 - \theta ,$$

or

$$\theta_2 = \theta_1 + 2\theta .$$

Taking Cartesian coordinates (x, y) in the vertical plane normal to the axes of the cylinders and through their centers of mass, as shown in Fig. 2.4, we have, at $t > 0$, for the lower cylinder

$$x_1 = -R\theta_1, \qquad y_1 = R ,$$

and for the upper cylinder

$$x_2 = x_1 + 2R\sin\theta ,$$
$$y_2 = 3R - 2(R - \cos\theta) = R + 2R\cos\theta .$$

The corresponding velocity components are

$$\dot{x}_1 = -R\dot{\theta}_1, \qquad \dot{y}_1 = 0 ,$$
$$\dot{x}_2 = -R\dot{\theta}_1 + 2R\dot{\theta}\cos\theta, \qquad \dot{y}_2 = -2R\dot{\theta}\sin\theta .$$

The kinetic energy of the lower cylinder is thus

$$T_1 = \frac{1}{2}M\dot{x}_1^2 + \frac{1}{4}MR^2\dot{\theta}_1^2 = \frac{3}{4}MR^2\dot{\theta}_1^2 ,$$

and that of the upper cylinder is

$$T_2 = \frac{1}{2}M(\dot{x}_2^2 + \dot{y}_2^2) + \frac{1}{4}MR^2\dot{\theta}_2^2$$

$$= \frac{1}{2}MR^2(\dot{\theta}_1^2 - 4\dot{\theta}_1\dot{\theta}\cos\theta + 4\dot{\theta}^2) + \frac{1}{4}MR^2(\dot{\theta}_1^2 + 4\dot{\theta}_1\dot{\theta} + 4\dot{\theta}^2)$$

$$= \frac{1}{4}MR^2[3\dot{\theta}_1^2 + 4\dot{\theta}_1\dot{\theta}(1 - 2\cos\theta) + 12\dot{\theta}^2] .$$

The potential energy of the system, taking the horizontal plane as level of reference, is

$$V = Mg(y_1 + y_2) = 2MR(1 + \cos\theta)g .$$

Hence the Lagrangian of the system is

$$L = T - V$$
$$= \frac{1}{2}MR^2[3\dot{\theta}_1^2 + 2\dot{\theta}_1\dot{\theta}(1 - 2\cos\theta) + 6\dot{\theta}^2] - 2MR(1 + \cos\theta)g .$$

Solution 2.2

(b) As only gravity is involved, the total mechanical energy of the system is a constant of the motion:

$$E = T + V$$
$$= \frac{1}{2}MR^2[3\dot{\theta}_1^2 + 2\dot{\theta}_1\dot{\theta}(1 - 2\cos\theta) + 6\dot{\theta}^2] + 2MR(1 + \cos\theta)g$$
$$= \text{ constant .}$$

Furthermore, if $\partial L/\partial q_i = 0$, Lagrange's equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

requires that $\partial L/\partial \dot{q}_i$ is conserved. For the system under consideration, $\partial L/\partial \theta_1 = 0$ so that

$$\frac{\partial L}{\partial \dot{\theta}_1} = MR^2[3\dot{\theta}_1 + \dot{\theta}(1 - 2\cos\theta)] = \text{ constant .}$$

Solution 2.3

$$L = \frac{1}{2}MR^2\left[3\dot{\theta}_1^2 + 2\dot{\theta}_1\dot{\theta}(1 - 2\cos\theta) + 6\dot{\theta}^2\right] - 2MR(1 - 2\cos\theta)g$$

Where θ_1 and θ are generalized coordinates

$$\Rightarrow P_{\theta_1} = \frac{dL}{d\dot{\theta}_1} = 3MR^2\dot{\theta}_1 + MR^2\dot{\theta}(1 - 2\cos\theta) \qquad\qquad \text{Eq. 1}$$

And

$$P_\theta = \frac{dL}{d\dot{\theta}} = MR^2\dot{\theta}_1(1 - 2\cos\theta) + 6MR^2\dot{\theta} \qquad\qquad \text{Eq. 2}$$

or, $\quad (1 - 2\cos\theta)P_{\theta_1} - 3P_\theta = \dot{\theta}\{ MR^2(1 - 2\cos\theta)^2 - 18MR^2\}$

$$\therefore \dot{\theta} = \frac{(1 - 2\cos\theta)P_{\theta_1} - 3P_\theta}{MR^2\{(1 - 2\cos\theta)^2 - 18\}} \qquad\qquad \text{Eq. 3}$$

or, $6P_{\theta_1} - (1 - 2\cos\theta)P_\theta = 18MR^2\dot{\theta}_1 - MR^2\dot{\theta}_1(1 - 2\cos\theta)^2 = MR^2\dot{\theta}_1\{18 - (1 - 2\cos\theta)^2\}$

$$\dot{\theta}_1 = \frac{(1 - 2\cos\theta)P_\theta - 6P_{\theta_1}}{MR^2\{(1 - 2\cos\theta)^2 - 18\}} \qquad\qquad \text{Eq. 4}$$

Now

$$H = \dot{\theta} \, P_\theta + \dot{\theta}_1 P_{\theta_1} - L \qquad\qquad \text{Eq. 5}$$

$$H = \dot{\theta}\, P_\theta + \dot{\theta}_1 P_{\theta_1} - \frac{1}{2} MR^2 \left[3\dot{\theta}_1{}^2 + 2\dot{\theta}_1\dot{\theta}(1 - 2\cos\theta) + 6\dot{\theta}^2\right] + 2MR(1 - 2\cos\theta)g \qquad \text{Eq. 6}$$

Now using the obtained values of $\dot{\theta}$ and $\dot{\theta}_1$ from Eq. 3&4

$$H = \frac{(1 - 2\cos\theta)P_{\theta_1} - 3P_\theta}{MR^2\{(1 - 2\cos\theta)^2 - 18\}} P_\theta + \frac{(1 - 2\cos\theta)P_\theta - 6P_{\theta_1}}{MR^2\{(1 - 2\cos\theta)^2 - 18\}} P_{\theta_1}$$
$$- \frac{1}{2}MR^2 \left[3\left(\frac{(1 - 2\cos\theta)P_\theta - 6P_{\theta_1}}{MR^2\{(1 - 2\cos\theta)^2 - 18\}}\right)^2 \right.$$
$$+ 2\left(\frac{(1 - 2\cos\theta)P_\theta - 6P_{\theta_1}}{MR^2\{(1 - 2\cos\theta)^2 - 18\}}\right)\left(\frac{(1 - 2\cos\theta)P_{\theta_1} - 3P_\theta}{MR^2\{(1 - 2\cos\theta)^2 - 18\}}\right)(1 - 2\cos\theta)$$
$$\left. + 6\left(\frac{(1 - 2\cos\theta)P_{\theta_1} - 3P_\theta}{MR^2\{(1 - 2\cos\theta)^2 - 18\}}\right)^2 \right] + 2MR(1 - 2\cos\theta)g$$

Solution 2.4

(c) As long as the cylinders remain in contact the results of (b) hold. Initially, $\theta = 0$, $\dot{\theta}_1 = \dot{\theta} = 0$, so that

$$\frac{1}{2}MR^2[3\dot{\theta}_1^2 + 2\dot{\theta}_1\dot{\theta}(1 - 2\cos\theta) + 6\dot{\theta}^2] + 2MR(1 + \cos\theta)g = 4MRg ,$$

$$MR^2[3\dot{\theta}_1 + \dot{\theta}(1 - 2\cos\theta)] = 0 .$$

These combine to give

$$\dot{\theta}^2[18 - (1 - 2\cos\theta)^2] = \frac{12}{R}(1 - \cos\theta)g ,$$

i.e.

$$\dot{\theta}^2 = \frac{12(1 - \cos\theta)g}{R(17 + 4\cos\theta - 4\cos^2\theta)} .$$

Solution Q 3

Sol. (i)

$$E(k) = E_o - 2\gamma \left[\cos(k_x a) + \cos(k_y a)\right] eV$$

This is the energy expression in 2D, i.e., for the square lattice with lattice parameter a. In the 1st Brillouin zone reciprocal unit cell, the top of the lowest band is at $(k_x, k_y) = \left[\pm\frac{\pi}{a}, \pm\frac{\pi}{a}\right]$ and the bottom of the band is at $(k_x, k_y) = (0, 0)$. Then,

$$\begin{aligned}
\text{Band Width} &= E_{top} - E_{bottom} \\
&= E_o + 2\gamma[1 + 1] - [E_o - 4\gamma] \\
&= 8\gamma \text{ eV}
\end{aligned}$$

(ii) Density of states in 2D is given by:

$$D_{2D}(E) = \frac{1}{L^2}\frac{dN}{dE}$$

For 2D case;

$$\frac{dN}{dE} = \frac{dN}{dk} \times \frac{dk}{dE} = \frac{kL^2}{\pi} \times \frac{dk}{dE}$$

Near the bottom of the band $ka \ll 1$. So,

$$\begin{aligned}
E(k) &\approx E_o - 2\gamma \left[1 - \frac{k_x^2 a^2}{2!} + 1 - \frac{k_y^2 a^2}{2!}\right] \\
&= E_o - 2\gamma \left[2 - \frac{a^2}{2}\left(k_x^2 + k_y^2\right)\right] \\
&= E_o - 4\gamma + \gamma a^2 \left(k_x^2 + k_y^2\right) = E_o - 4\gamma + \gamma a^2 k^2
\end{aligned}$$

Now,

$$\begin{aligned}
\frac{dE}{dk} &= 2\gamma a^2 k \\
\Rightarrow \frac{dk}{dE} &= \frac{1}{2\gamma a^2 k}
\end{aligned}$$

Then,

$$D_{2D}(E) = \frac{1}{L^2} \frac{kL^2}{\pi} \times \frac{1}{2\gamma a^2 k}$$

$$= \frac{1}{2\pi\gamma a^2}.$$

(iii) Wave velocity (group velocity) near the centre of the Brillouin zone:

$$v_g = \frac{1}{\hbar} \frac{dE}{dk}$$

$$\Rightarrow v_g = \frac{2\gamma a^2 k}{\hbar}.$$

(iv) Effective mass at the bottom of the band, i.e., at $(k_x, k_y) = (0, 0)$ is:

$$m^* = \frac{\hbar^2}{\dfrac{d^2 E}{dk^2}}$$

$$= \frac{\hbar^2}{2\gamma a^2}$$

And,

Effective mass at the top of the band $= -$(Effective mass at the bottom of the band)

$$= -\frac{\hbar^2}{2\gamma a^2}$$

Solution Q 4.1

Solution: Concentration of silicon atoms= $5 \times 10^{24} atoms/cm^3$

Because doping is done at 2 atoms per 10^8 silicon atoms.

$$N_A = \frac{2 \times 5 \times 10^{24}}{10^8} = 10^{17}/cm^3$$

$$N_V = 2\left(\frac{2\pi m_p KT}{h^2}\right)^{\frac{3}{2}}$$

K=Boltzman's constant in $eV/°K$; $\underline{K}$= Boltzmann's constant in $J/°K$.

h= Planck's constant=6.62×10^{-34} J-sec

$\underline{K} = 1.38 \times 10^{-23} J/°K$

$$N_V = 2\left(\frac{2\pi m_p \underline{KT}}{h^2}\right)^{\frac{3}{2}} = 4.82 \times 10^{21} \left(\frac{m_p}{m_e}\right)^{\frac{3}{2}} T^{\frac{3}{2}}$$

Where $m_p = 0.7 m_e$ (given)

$$T = 290\ K$$

$$N_V = 4.82 \times 10^{21}(0.7 \times 290)^{\frac{3}{2}} = 1.3940 \times 10^{25}/m^3 = 1.3940 \times 10^{19}/cm^3$$

$$E_F - E_V = KTln(N_V/N_A)$$

$$= 0.025ln\left(\frac{1.3940 \times 10^{19}}{10^{17}}\right)$$

$$= 0.123\ eV$$

Or $E_F - E_V = 0.123\ eV$

$\therefore E_F$ is above E_V.

Solution 4.2

Conductivity of a material is determined by two factors: the concentration of free carriers available to conduct current and their mobility (or freedom to move). In a semiconductor, both mobility and carrier concentration are temperature dependent. Thus, it is important to view the conductivity as a function of temperature which is expressed by:

$$\sigma = q\left[\mu_n(T)n(T) + \mu_p(T)p(T)\right] \quad (2)$$

There are two basic types of scattering mechanisms that influence the mobility of electrons and holes: lattice scattering and impurity scattering. We have already discussed lattice scattering in the context of metals; we know that lattice vibrations cause the mobility to decrease with increasing temperature.

However, the mobility of the carriers in a semiconductor is also influenced by the presence of *charged impurities*. Impurity scattering is caused by crystal defects such as ionized impurities. A lower temperatures, carriers move more slowly, so there is more time for them to interact with charged impurities. As a result, as the temperature decreases, impurity scattering *increases*, and the mobility *decreases*. This is just the opposite of the effect of lattice scattering.

The total mobility then is the sum of the lattice-scattering mobility and the impurity-scattering mobility. Figure 1 shows how the total mobility has a temperature at which it is a maximum. The approximate temperature dependence of mobility due to lattice scattering is $T^{-3/2}$, while the temperature dependence of mobility due to impurity scattering is $T^{+3/2}$ (see Figure 1). In practice, impurity scattering is typically only seen at very low temperatures. In the temperature range we will measure, only the influence of lattice scattering will be expected.
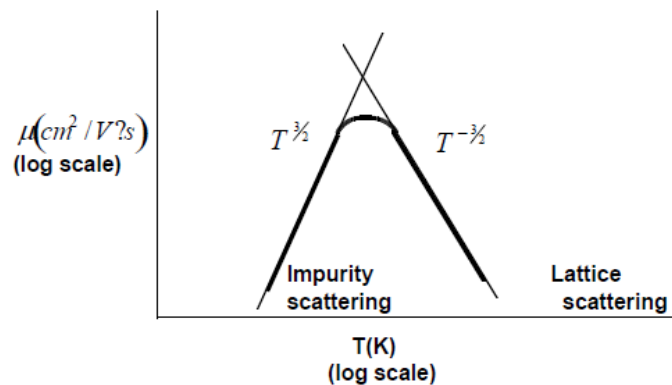
We know that

$$p = N_v e^{-\frac{E_f - E_v}{kT}}$$

After putting the value of given in question

We get

$$p = 9.84 \times 10^{18} \times e^{-\frac{0.123 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} \times 300}}$$

$$p = 8.5 \times 10^{16} \ /cm^3$$