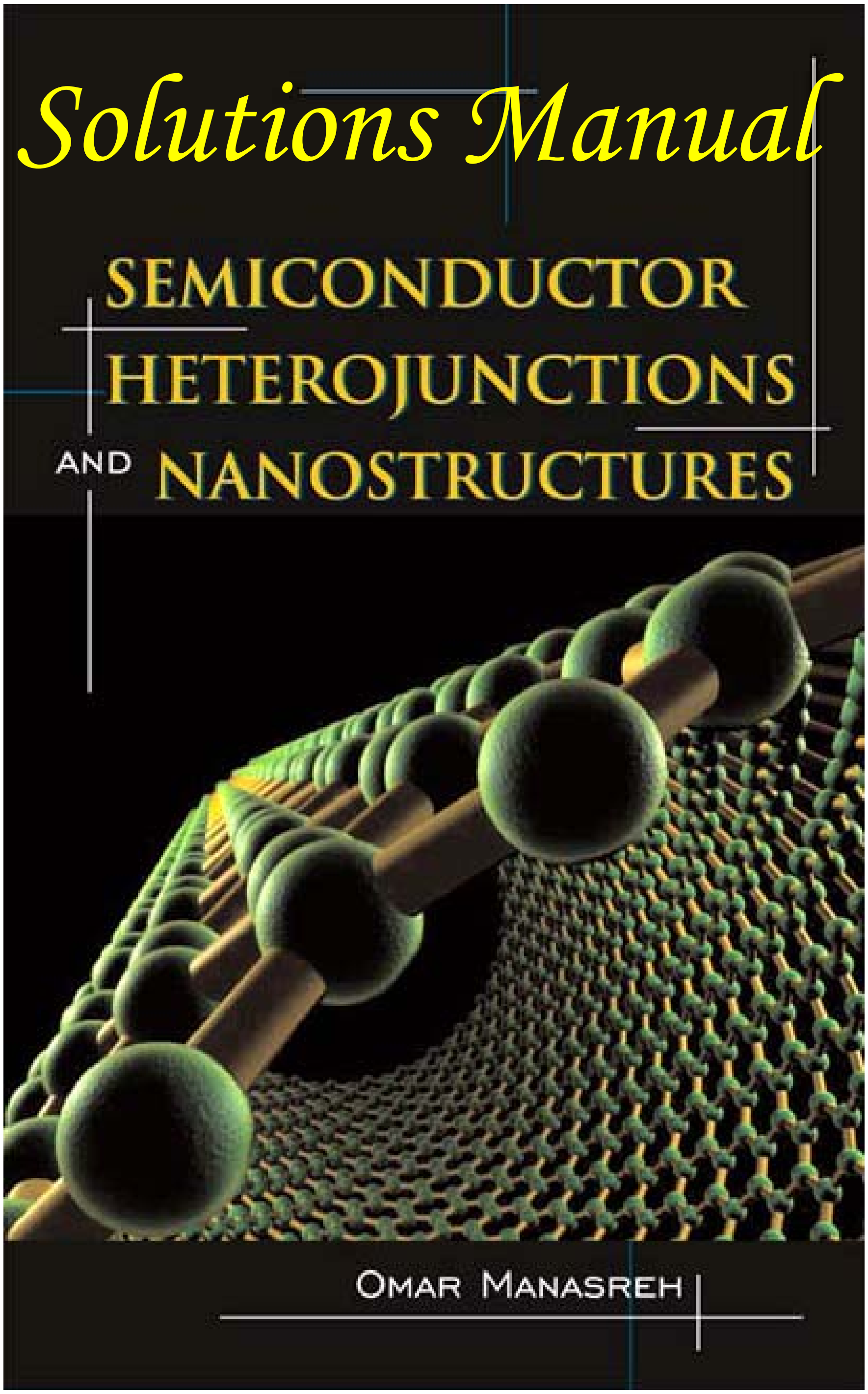


McGraw-Hill
New York, 2005

Problems and Solution
Chapter One

1.1 Show that the total internal energy per oscillator for a system of 3N oscillators is $U = k_B T$. Start with Dulong and Petit model.

Solution:

Using Dulong and Petit assumtion along with Maxwell-Boltzman distribution function, one can write

$$U = \frac{\overline{E}}{3N} = \frac{\int_0^\infty E e^{-E/k_B T} dE}{\int_0^\infty e^{-E/k_B T} dE}; \text{ where } \overline{E} \equiv \text{ total energy of the system}$$

$$U = \frac{e^{-E/k_B T}\left[\frac{E}{-1/(k_B T)} - \frac{1}{-1/(k_B T)}\right]_0^\infty}{\left[-\frac{e^{-E/k_B T}}{-1/(k_B T)}\right]_0^\infty}$$

$$= \frac{0 - \left(\frac{-1}{-1/(k_B T)^2}\right)}{\frac{1}{-1/(k_B T)}[0-1]} = \frac{(k_B T)^2}{(k_B T)} = k_B T$$

1.2 Derive Einstein's expression for the specific heat capacity of solid given by Eq. (1.8).

Solution: Einstein assumed that each atom is a single harmonic oscillator with energy given by $E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega$. By using Maxwell-Boltzmann distribution function, we have

$$E = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_B T}}{\sum_{n=0}^{\infty} e^{-E_n/k_B T}}; \quad \text{assuming that each energy level is a non-degenerate}$$

$$= \frac{\hbar\omega \sum_{n=0}^{\infty}\left(n+\tfrac{1}{2}\right) e^{-x\left(n+\frac{1}{2}\right)}}{\sum_{n=0}^{\infty} e^{-x\left(n+\frac{1}{2}\right)}}; \quad \text{where } x = -\frac{\hbar\omega}{k_B T}$$

$$= \frac{\hbar\omega\left[\tfrac{1}{2}e^{\frac{1}{2}x} + \tfrac{3}{2}e^{\frac{3}{2}x} + \tfrac{5}{2}e^{\frac{5}{2}x} + ...\right]}{\left[e^{\frac{1}{2}x} + e^{\frac{3}{2}x} + e^{\frac{5}{2}x} + ...\right]}$$

$$= \frac{d}{dx}\left[e^{\frac{1}{2}x}\left(1 + e^{x} + e^{2x} + ...\right)\right] = \hbar\omega \frac{d}{dx}\left[\tfrac{1}{2}x + \ln(1 - e^{x})\right]$$

$$= \tfrac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

$$C_v = \frac{\partial E}{\partial T} = \frac{\partial\left(\tfrac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}\right)}{\partial T} = \hbar\omega \frac{\partial\left(e^{\hbar\omega/k_B T} - 1\right)^{-1}}{\partial T}$$

$$= -\hbar\omega\left(e^{\hbar\omega/k_B T} - 1\right)^{-2} \frac{\partial e^{\hbar\omega/k_B T}}{\partial T} = -\hbar\omega\left(e^{\hbar\omega/k_B T} - 1\right)^{-2} e^{\hbar\omega/k_B T} \frac{\hbar\omega}{k_B} \frac{\partial(T^{-1})}{\partial T}$$

$$= \frac{-\hbar\omega e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2} \frac{\hbar\omega}{k_B} \frac{(-1)}{T^2}$$

$$= k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2}; \quad \text{Let } \Theta_E = \hbar\omega/k_B; \text{ then we have}$$

$$C_v = k_B \left(\frac{\Theta_E}{T}\right)^2 \frac{e^{\frac{\Theta_E}{T}}}{\left(e^{\frac{\Theta_E}{T}} - 1\right)^2}. \quad \text{For 3N particles, we have}$$

$$C_v = 3Nk_B \left(\frac{\Theta_E}{T}\right)^2 \frac{e^{\frac{\Theta_E}{T}}}{\left(e^{\frac{\Theta_E}{T}} - 1\right)^2}$$

1.3 The work function of a material is the minimum energy required to remove an electron from the surface of the material. Calculate the maximum wavelength of light for the photoelectric emission from gold (φ_o=4.90V) and cesium (φ_o=1.90V).

Solution: Photoelectric emission requires that the photon energy is equal to the threshold energy needed to remove an electron from the surface of the material

$$\varphi_o = 4.9V \text{ for gold } \Rightarrow e\varphi_o = 4.9V$$

$$\varphi_o = 1.9V \text{ for cesium } \Rightarrow e\varphi_o = 1.9V$$

$$E = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E}$$

$$For \text{ gold: } \lambda = \frac{\left(6.625\times10^{-34}\right)\left(3\times10^{10}\right)}{\left(4.9\right)\left(1.6\times10^{-19}\right)} = 0.254\mu m = 254nm$$

$$For \text{ cecium: } \lambda = \frac{\left(6.625\times10^{-34}\right)\left(3\times10^{10}\right)}{\left(1.9\right)\left(1.6\times10^{-19}\right)} = 0.654\mu m = 654nm$$

1.4 Use the uncertainty relation to evaluate the ground state of the hydrogen atom.

Solution: Uncertainty principle tells us that $\Delta p \Delta r \approx \hbar$. Assume that $\Delta r = r_o$ = radius of the electron orbit in the hydrogen atom. For the electron-proton system, we have

$$E = \frac{P^2}{2m} V(r); \quad \text{where } p^2 = \frac{\hbar^2}{r_0^2} \text{ and } V(r) = -\frac{e^2}{4\pi\epsilon_o r_o}$$

$$\therefore E = \frac{\hbar^2}{2mr_0^2} - \frac{e^2}{4\pi\epsilon_o r_o}; \text{ For a minimum value of } E(r_o), \text{ the first derivative of } E \text{ with trespect to } r_o \text{ should be zero.}$$

$$\Rightarrow \frac{\partial E}{\partial r_o} = 0 = \frac{\partial}{\partial r_o}\left[\frac{\hbar^2}{2mr_0^2} - \frac{e^2}{4\pi\epsilon_o r_o}\right] = \frac{\hbar^2}{2m}\frac{\partial}{\partial r_o}\left[\frac{1}{r_0^2}\right] - \frac{e^2}{4\pi\epsilon_o}\frac{\partial}{\partial r_o}\left[\frac{1}{r_0}\right] = -\frac{\hbar^2}{2m}\frac{1}{r_0^3} - \frac{(-1)e^2}{4\pi\epsilon_o}\frac{1}{r_0^2}$$

$$\therefore r_o = \frac{4\pi\epsilon_o\hbar^2}{me^2}$$

$$= \frac{4\,\pi\left(6.65\times10^{-12} F/m\right)\left(1.055\times1-^{-34}\, J.s\right)^2}{\left(9.1\times10^{-31}kg\right)\left(1.6\times10^{-19}C\right)^2} = 5.24\times10^{-11} m = 0.424 Angstrom$$

$$\textit{Substitute} \text{ the expression of } r_o \text{ into } E \text{ to obtain } E = -\frac{me^4}{\left(4\pi\epsilon_o\hbar\right)^2}$$

$$\therefore E = -\frac{\left(9.1\times10^{-31}kg\right)\left(1.6\times10^{-19}C\right)^4}{\left(4\,\pi\times6.65\times10^{-12}F/m\right)^2\left(1.055\times10^{-34}J.s\right)^2} = -2.16\times10^{-18} J = -13.3 eV$$

1.5 Calculate the de Broglie wavelength for (a) an electron with kinetic energy of 10^4eV, (b) a proton of kinetic energy of 10^2 eV, and a (150kg) man running at a speed of 0.25m/s.

Solution:

(a)

λ for an electron with a kinetic energy of 10^4 eV, we have

$$E_{K.E.} = \frac{P^2}{2m} \Rightarrow p = \sqrt{2mE_{K.E.}} = \sqrt{2(9.11\times10^{-31}kg)(10^4\times1.6\times10^{-19}J)} = 5.399\times10^{-23}kg.m/s$$

$$\lambda = \frac{h}{p} = \frac{2\pi\times1.055\times10^{-34}}{5.399\times10^{-23}} = 1.228 Angstrom$$

(b) For a proton, we have

λ for a proton with a kinetic energy of 10^2 eV, we have

$$E_{K.E.} = \frac{P^2}{2m} \Rightarrow p = \sqrt{2mE_{K.E.}} = \sqrt{2(1.67\times10^{-27}kg)(10^2\times1.6\times10^{-19}J)} = 2.312\times10^{-22}kg.m/s$$

$$\lambda = \frac{h}{p} = \frac{2\pi\times1.055\times10^{-34}}{2.312\times10^{-23}} = 0.02868 Angstrom$$

(c) For a man, we have:

The momentum of the man is $p = m\upsilon = 150kg\times0.24m/s = 37.5kg.m/s$

$$\lambda = \frac{h}{p} = \frac{2\pi\times1.055\times10^{-34}}{37.7} = 1.768\times10^{-25} Angstrom$$

1.6 Start from Eq. (1.35), write the Fourier transform of this wave function in term of g(ω). Then assume that $g(\omega)=|g(\omega)|e^{i\beta(\omega)}$. Derive the uncertainty principle presented in Eq. (1.37).

Solution:

$\psi(r,t) = Ae^{i\omega t}$ or $\psi(0,t) = Ae^{i\omega t}$.

The Fourier-transform of the function is

$$\psi(r,t) = \frac{1}{\sqrt{2\pi}}\int e^{i\omega t} g(\omega)d\omega \;;\quad \text{where A}=\frac{1}{\sqrt{2\pi}}$$

The inverse of the Fourier transform is

$$\psi(r,t) = \frac{1}{\sqrt{2\pi}}\int \psi(0,t)e^{i\omega t}dt \;;\quad \text{where g}(\omega)=|\text{g}(\omega)|e^{i\beta(t)}$$

The introduced variable $\beta(\omega)$ varies smoothly in the interval $[\omega_o - \Delta\omega/2,\ \omega_o + \Delta\omega/2\ ]$, where g($\omega$) is appreciable. For small $\Delta\omega/2$, $\beta(\omega)$ can be expanded as

$$\beta(\omega) \approx \beta(\omega_o) + (\omega-\omega_o)\left.\frac{d\beta(\omega)}{d\omega}\right|_{\omega=\omega_o} + ...$$

Let $t_o = -\left.\frac{d\beta(\omega)}{d\omega}\right|_{\omega=\omega_o}$

$$\therefore \beta(\omega) \approx \beta(\omega_o) - (\omega-\omega_o)t_o$$

$$\psi(0,t) \approx \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}|g(\omega)|e^{i\{\beta(\omega_o)-(\omega-\omega_o)t_o\}}e^{i\omega t}d\omega = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}|g(\omega)|e^{i\{\beta(\omega_o)-\omega t_o-\omega_o t_o\}}e^{i\omega t}\cdot e^{+i\omega_o t}\cdot e^{-i\omega_o t}d\omega$$

$$= \frac{e^{i\{\beta(\omega_o)+\omega_o t\}}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}|g(\omega)|e^{i\{-\omega t_o+\omega_o t_o\}}e^{i\omega t}\cdot e^{-i\omega_o t}d\omega = \frac{e^{i\{\beta(\omega_o)+\omega_o t\}}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}|g(\omega)|e^{i\{\omega(t-t_o)-\omega_o(t-t_o)\}}d\omega$$

$$\therefore \psi(0,t) \approx \frac{e^{i\{\beta(\omega_o)+\omega_o t\}}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}|g(\omega)|e^{i(\omega-\omega_o)(t-t_o)}d\omega$$

The function $e^{i(\omega-\omega_o)(t-t_o)}$ oscillate approximately once when $(\omega-\omega_o)(t-t_o)\approx 1$.

Or $\Delta\omega\Delta t \approx 1 \Rightarrow \hbar\Delta\omega\Delta t \approx \hbar \quad \Rightarrow \Delta E\Delta t \geq \hbar$.

1.7 Show that Δp.Δx ~ ΔE.Δt.

Solution:

$$\Delta E = \frac{dE}{dp}.dp = \frac{dE}{dp}.\Delta p$$

From Planck and Einstein relations we have

$E = \hbar\omega$ and $p = \hbar k$; where k is the wave verctor

$$Then\ \frac{dE}{dp} = \frac{d\hbar\omega}{d\hbar k} = \frac{d\omega}{dk} = \upsilon_g;$$ where υ_g is the group velocity

$\therefore$ ΔE=$\upsilon_g \Delta p$.

The charcteristic evolution time, Δt, is the time taken by the wave packet traveling with a group velocity. υ_g, to pass a point in space. If Δx is the spatial extension of the wave packet, then we have

$$\Delta t \approx \frac{\Delta x}{\upsilon_g} \text{ or } \upsilon_g \approx \frac{\Delta x}{\Delta t} \Rightarrow \Delta E = \upsilon_g \Delta p = \frac{\Delta x}{\Delta t}\Delta p$$

$$or\ \ \Delta E \Delta t = \Delta x \Delta p$$

1.8 If $|\psi\rangle$ can be normalized to unity and assume that an operator **A**=$|\psi\rangle\langle\psi|$. Show that **A**^{2}=**A**

Solution:

$|\psi\rangle$ can be normalized to 1 or $\langle\psi|\psi\rangle = 1$

$$A = |\psi\rangle\langle\psi|$$

$$A^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle(\langle\psi|\psi\rangle)\langle\psi| = |\psi\rangle(1)\langle\psi| = |\psi\rangle\langle\psi| = A$$

1.9 Assume that *[X,P]=i ħ*. Show that *[X,P^2]=2i ħ P*, then show that *[X,P^n]=i ħnP^{n-1}*.

Solution:

$$\left[X,P\right]=i\hbar$$

$$\left[X,P^2\right]=\left[X,PP\right]=XPP-PPX = XPP-PPX - XPX + PXP$$

$$=\left(\text{XPP-PXP}\right)+\left(\text{PXP-PPX}\right)=\left[X,P\right]P+P\left[X,P\right]=2\left[X,P\right]P=2i\hbar P$$

Assume that $\left[X,P^n\right]=i\hbar nP^{n-1}$ is correct, then $\left[X,P^n\right]$ can be induced by working with $\left[X,P^{n+1}\right]$.

$$\left[X,P^{n+1}\right]=\left[X,PP^n\right]=XPP^n-PP^nX = XPP^n-PP^nX-PXP^n+PXP^n$$

$$=XPP^n-PXP^n+PXP^n-PP^nX = \left[X,P\right]P^n+P\left[X,P^n\right]$$

$$=i\hbar P^n+Pni\hbar P^{n-1}=i\hbar P^n+ni\hbar P^n = (n+1)i\hbar P^n$$

$\therefore\left[X,P^{n+1}\right]=(n+1)i\hbar P^n$ therefore $\left[X,P^n\right]=(n+1)i\hbar P^{n-1}$

1.10 Care must be taken when working with operator. The order of the operator is very important. Assume that **A** and **B** are operators that do not commute. Show that $e^{\mathbf{A}}e^{\mathbf{B}}$, $e^{\mathbf{B}}e^{\mathbf{A}}$, and $e^{\mathbf{A+B}}$ are not equal.

Solution:

$$e^A=\sum_p\frac{A^p}{p!} \quad and \quad e^B=\sum_q\frac{B^q}{q!} \quad where\ p\neq q$$

$$e^Ae^B=\sum_p\frac{A^p}{p!}\sum_q\frac{B^q}{q!}=\sum_{p,q}\frac{A^pB^q}{p!q!}$$

Similarly:

$$e^Be^A=\sum_{q,p}\frac{B^qA^p}{q!p!}\ ; \quad Also\ e^{A+B}=\sum_p\frac{\left(A+B\right)^p}{p!}$$

It is clear that none of these quantities are equal.

If A and B commute, then

$$[A,B]=0 \Rightarrow e^Ae^B=e^Be^A=e^{A+B}=e^{B+A}$$

1.11 A series of lines in hydrogen correspond to transitions to a final state characterized by some quantum number n. If the wavelength of the radiation giving rise to the first line is 657 nm, what are the wavelengths corresponding to the next two lines. Assume that Δn=1.

Solution:

$$\frac{hc}{\lambda} = \tfrac{1}{2} m_e c^2 \alpha^2 \left(\frac{1}{n_l^2} - \frac{1}{n_z^2} \right);\ \ m_e c^2 = 0.51 \times 10^6 \text{ eV and hc=, } \alpha = 1/137$$

$$\therefore \frac{1}{657 \times 10^{-9} m} = \frac{0.5\left(0.51 \times 10^6 \text{ eV}\right)\left(1/137\right)^2}{1.24 \times 10^{-6} \text{ eV-m}} \left(\frac{1}{n^2} - \frac{1}{(n+1)^2} \right)$$

$$\left(\frac{1}{n^2} - \frac{1}{(n+1)^2} \right) = 0.139$$

$$\frac{1}{\lambda} = 1.096 \times 10^7 \left(\frac{1}{n^2} - \frac{1}{(n+1)^2} \right)$$

$$For \text{ n=1 we have } \left(\frac{1}{n^2} - \frac{1}{(n+1)^2} \right) = 0.75 \ \Rightarrow \lambda\text{=121.7 nm}$$

$$For \text{ n=2 we have } \left(\frac{1}{n^2} - \frac{1}{(n+1)^2} \right) = 0.139 \ \Rightarrow \lambda\text{=657 nm}$$

$$For \text{ n=3 we have } \left(\frac{1}{n^2} - \frac{1}{(n+1)^2} \right) = 0.75 \ \Rightarrow \lambda\text{=1876.96 nm}$$

1.12 Show that the integration of a δ-function is a step function.

Solution:

Assume that $\delta^{(\varepsilon)}(x) = \begin{cases} 1/\varepsilon & \text{for } -\frac{\varepsilon}{2} < x < +\frac{\varepsilon}{2} \\ 0 & \text{for } x \le -\frac{\varepsilon}{2} \text{ and } x \ge +\frac{\varepsilon}{2} \end{cases}$

Let $\theta^{(\varepsilon)}(x) = \int_{-\infty}^{x} \delta^{(\varepsilon)}(x')dx'$ where x' is a variable

for $x \le -\frac{\varepsilon}{2}$ $\delta^{(\varepsilon)}(x) = 0$ and $\theta^{(\varepsilon)}(x) = \int_{-\infty}^{\infty} 0dx' = 0$

for $x \ge +\frac{\varepsilon}{2}$ we have $\int_{-\infty}^{\frac{\varepsilon}{2}} \delta^{(\varepsilon)}(x')dx' = 1$, definition of the δ-function

$\therefore \theta^{(\varepsilon)}(x) = 1$ for $x \ge +\frac{\varepsilon}{2}$

or $-\frac{\varepsilon}{2} < x < +\frac{\varepsilon}{2}$, we have $\delta^{(\varepsilon)} = \frac{1}{\varepsilon}$, which gives

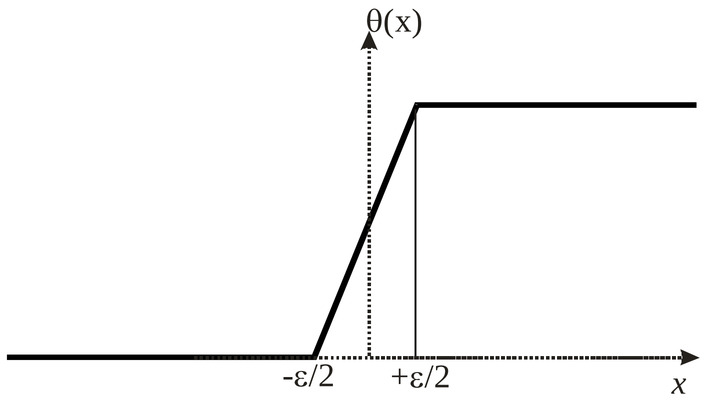
$\theta^{(\varepsilon)}(x) = \int_{-\infty}^{x} \delta^{(\varepsilon)}(x')dx' = \int_{-\frac{\varepsilon}{2}}^{x} \frac{1}{\varepsilon}dx' = \frac{1}{\varepsilon}x\Big|_{-\frac{\varepsilon}{2}}^{x} = \frac{1}{\varepsilon}\left(x + \frac{\varepsilon}{2}\right)$

The variation of $\theta^{(\varepsilon)}(x)$ is shown in the figure.

As $\varepsilon \to 0$ we have $\frac{1}{\varepsilon}\left(x + \frac{\varepsilon}{2}\right)$, *where* $x \to \frac{\varepsilon}{2}$ and $\frac{1}{\varepsilon}\left(x + \frac{\varepsilon}{2}\right) \to 1$

Thus, $\theta^{(\varepsilon)}(x) = \begin{cases} 1 & \text{for x<0} \\ 0 & \text{for x>0} \end{cases}$ Heaviside step function

Again, the derivative of $\theta^{(\varepsilon)}(x)$ is δ-function.



1.13 Derive the expression of Fourier transform function shown in Eq. (1.98).

Solution:

Let $\psi_{\mathrm{L}}(x)$ to be the periodic function of L, which is equal to $\psi(x)$ inside the interval $\left[-\frac{\mathrm{L}}{2},+\frac{\mathrm{L}}{2}\right]$. $\psi_{\mathrm{L}}(x)$ can be expanded in Fourier series as shown in Eq. (1.94)

$$\psi_{\mathrm{L}}(x)=\sum_{n=-\infty}^{\infty} C_n e^{ik_n x}, \quad \text{where } k_n = n\frac{2\pi}{L} \quad \text{and}$$

$$C_n = \int_{x_o}^{x_o+L} dx e^{-ik_n x}\psi_{\mathrm{L}}(x) = \frac{1}{L}\int_{-L/2}^{L/2} dx e^{-ik_n x}\psi(x); \quad \text{when } \mathrm{L}\to\infty, \text{ then } \psi_{\mathrm{L}}(x)\to\psi(x)$$

Notice that $k_{n+1} - k_n = (n+1)\frac{2\pi}{L} - n\frac{2\pi}{L} = \frac{2\pi}{L}$, or $\frac{1}{\mathrm{L}} = \frac{k_{n+1} - k_n}{2\pi}$

$$\therefore C_n = \frac{k_{n+1} - k_n}{2\pi}\int_{-L/2}^{L/2} dx e^{-ik_n x}\psi(x); \quad \text{substitute } C_n \text{ into } \psi_{\mathrm{L}}(x) \text{ to obtain}$$

$$\psi_{\mathrm{L}}(x) = \sum_{n=-\infty}^{\infty} \frac{k_{n+1} - k_n}{2\pi} e^{ik_n x}\int_{-L/2}^{L/2} dx' e^{-ik_n x'}\psi(x')$$

When $\mathrm{L}\to\infty$, then $(k_{n+1} - k_n)\to 0$, thus the sum over n can be transformed into a definite integral and $\psi_{\mathrm{L}}(x)\to\psi(x)$.

Let us set $\overline{\psi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-L/2}^{L/2} dx' e^{-ik_n x'}\psi(x')$

Change summation to integral, we have

$$\psi_{\mathrm{L}}(x) = \psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\overline{\psi}(k)dk$$

Now, $p = \hbar k \Rightarrow dk = \frac{dp}{\hbar}$ or

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\,\overline{\psi}(p)dp; \quad \text{notice that we set } \overline{\psi}(p) = \frac{1}{\sqrt{\hbar}}\overline{\psi}(k) = \frac{1}{\sqrt{\hbar}}\overline{\psi}(p/\hbar)$$

The inverse of the Fourier transform is

$$\overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\,\psi(x)dx$$

1.14 If $A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, write an expression for e^A in a matrix form.

Solution:

$$A = \begin{pmatrix} e^{1} & e^{0} \\ e^{0} & e^{-1} \end{pmatrix};\ e^{A} = e^{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}} = \begin{pmatrix} e^{1} & e^{0} \\ e^{0} & e^{-1} \end{pmatrix} = \begin{pmatrix} e & 1 \\ 1 & 1/e \end{pmatrix}$$

This can be diagonalized to

$$\begin{pmatrix} e & 0 \\ 0 & 1/e \end{pmatrix}$$

1.15 Show that $\sum_j |u_j\rangle\langle u_j| = 1$. This is called the closure relation.

Solution:

$|\psi\rangle = \sum_i C_i |u_i\rangle$, This is called Fourier series

Apply $\langle u_j|$ to both side

$$\langle u_j|\psi\rangle = \sum_i \langle u_j|C_i|u_i\rangle = C_j$$

$$\therefore |\psi\rangle = \sum_i C_i|u_i\rangle = |\psi\rangle = \sum_i \langle u_j|\psi\rangle|u_i\rangle = \sum_i |u_i\rangle\langle u_j|\psi\rangle = \left(\sum_i |u_i\rangle\langle u_j|\right)|\psi\rangle$$

$1 = \sum_i |u_i\rangle\langle u_j|$; This is called unity or identity operator.

1.16 Find the Fourier transform of the following functions:

(a) $\overline{\psi}(x) = \frac{1}{a}$ for $-\frac{a}{2} < x < \frac{a}{2}$

$=0$ for $|x| > \frac{a}{2}$

(b) $\psi(x) = e^{-ax}$ for $x>0$

$= 0$ for $x<0$

(c) $\psi(x) = e^{-x^2/a^2}$

Solution:

(a) $$\overline{\psi}(x) \Rightarrow \overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \psi(x) dx$$

$$\overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-a/2}^{a/2} e^{ipx/\hbar} \frac{1}{a} dx = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{a} \frac{e^{ipx/\hbar}}{ip/\hbar}\Bigg|_{-a/2}^{a/2} = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{iap/\hbar} e^{ipx/\hbar}\Big|_{-a/2}^{a/2}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{2}{ap/\hbar} \frac{1}{2i}\left(e^{ipa/2\hbar} - e^{-ipa/2\hbar}\right) = \frac{1}{\sqrt{2\pi\hbar}} \frac{\sin(pa/2\hbar)}{ap/\hbar}$$

Since $\overline{\psi}(x) = \frac{1}{a}$ for $-\frac{a}{2} < x < \frac{a}{2}$

$=0$ for $|x| > \frac{a}{2}$

Then $\overline{\psi}(x)$ has a form of δ-function. Thus the Fourier transform of a δ-function is simply a sinc-function

(b) $$\overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{0}^{\infty} e^{-ipx/\hbar} e^{-x/a} dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{0}^{\infty} e^{-ipx/\hbar - x/a} dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{0}^{\infty} e^{-ipx/\hbar - x/a} dx = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(ip/\hbar - 1/a)} e^{-ipx/\hbar - x/a}\Big|_{0}^{\infty} = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(-ip/\hbar - 1/a)}(0-1)$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(ip/\hbar + 1/a)}$$

Multiply this expression by $\frac{(ip/\hbar - 1/a)}{(ip/\hbar - 1/a)}$ to obtain the real part of the function as

Real $\overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1/a}{\left((p/\hbar)^2 + (1/a)^2\right)}$. This is a Lorentzian lineshape.

(c) $$\psi(x) = e^{-x^2/a^2} \Rightarrow \overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} e^{-x^2/a^2} dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{\infty}^{\infty} e^{-ipx/\hbar - x^2/a^2} dx$$

$\overline{\psi}(p) = \frac{a}{\sqrt{2\pi\hbar}} e^{-p^2a^2/4\hbar^2}$, which is a Guassian function.

1.17 Show that the second order perturbation Schrödinger Equation is given by (1.117). Project this equation onto the wave vectors $|\varphi_n\rangle$ to obtain the final expression $E_n(\lambda)$ to the second order as shown in (1.132).

Solution:

Start from Schordinger equation:

$$\left(H_o + \lambda \widehat{H}_1\right)\sum_n \lambda^n |n\rangle = \sum_{n'} \lambda^{n'} E_{n'} \sum_n \lambda^n |n\rangle$$

Second order approxiamtion yields

$$\left(H_o + \lambda \widehat{H}_1\right)\left(|0\rangle + \lambda|1\rangle + \lambda^2|2\rangle\right) = \left(E_o + \lambda E_1 + \lambda^2 E_2\right)\left(|0\rangle + \lambda|1\rangle + \lambda^2|2\rangle\right)$$

$$H_o|0\rangle + \lambda H_o|1\rangle + \lambda^2 H_o|2\rangle + \lambda\widehat{H}_1|0\rangle + \lambda^2\widehat{H}_1|1\rangle + \lambda^3\widehat{H}_1|2\rangle = E_o|0\rangle + \lambda E_o|1\rangle + \lambda^2 E_o|2\rangle + \lambda E_1|0\rangle + \lambda^2 E_1|1\rangle$$
$$+\lambda^3 E_1|2\rangle + \lambda^2 E_2|0\rangle + \lambda^3 E_2|1\rangle + \lambda^4 E_2|2\rangle$$

We concerned with the coefficient of λ^2. Thus, by ignoring all terms other than thos with λ^2, we have

$$H_o|2\rangle + \widehat{H}_1|1\rangle = E_o|2\rangle + E_1|1\rangle + E_2|0\rangle + O\left(\lambda^3\right)$$

or $\left(H_o - E_o\right)|2\rangle + \left(\widehat{H}_1 - E_1\right)|1\rangle - E_2|0\rangle = 0.$

Pr*oject* this equation onto $|\varphi_n\rangle$, we have

$$\langle\varphi_n|\left(H_o - E_o\right)|2\rangle + \langle\varphi_n|\left(\widehat{H}_1 - E_1\right)|1\rangle - E_2\langle\varphi_n|0\rangle = 0$$

Recall that $\langle\varphi_n| = \langle 0| \Rightarrow \langle\varphi_n|0\rangle = 1$. Let $\mathrm{H_o}$ operate on $\langle\varphi_n|$, which renders the first term zero.

Also $E_1\langle\varphi_n|1\rangle = 0$ since $\langle\varphi_n|$ and $\langle 1|$ are orthogonal.

$$\therefore \langle\varphi_n|\left(\widehat{H}_1\right)|1\rangle = E_2$$

From the first order perturbation we have

$|1\rangle = \sum_{u\neq n}\sum_i \frac{\langle\varphi_u^{'}|\left(\widehat{H}_1\right)|\varphi_n\rangle}{E_n^o - E_u^o}|\varphi_u^{'}\rangle$. Substitute this ket into the above equation to obtain

$$E_2 = \langle\varphi_n|\left(\widehat{H}_1\right)\sum_{u\neq n}\sum_i \frac{\langle\varphi_u^{'}|\left(\widehat{H}_1\right)|\varphi_n\rangle}{E_n^o - E_u^o}|\varphi_u^{'}\rangle = \sum_{u\neq n}\sum_i \frac{\left|\langle\varphi_u^{'}|\left(\widehat{H}_1\right)|\varphi_n\rangle\right|^2}{E_n^o - E_u^o}.$$

By including the first and second order perturbations, the energy can be written as

$$E_n = E_o + \langle\varphi_n|H_1|0\rangle + \sum_{u\neq n}\sum_i \frac{\left|\langle\varphi_u^{'}|H_1|\varphi_n\rangle\right|^2}{E_n^o - E_u^o}$$