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# Basic Quantum Mechanics

### 3.1 SCHRÖDINGER EQUATION

$$H\psi(\mathbf{r}, t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t)$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)$$

For a free particle V(r, t ) = 0, the solution is simply a plane wave:

$$\psi(\mathbf{r}, t) = \frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r} - \mathrm{i}Et/\hbar} \qquad E = \frac{\hbar^2 k^2}{2m}$$

The probability density is defined as $\rho(\mathbf{r}, t) = \psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t)$

probability current density as $\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2mi}[\psi^*\nabla\psi - \psi\nabla\psi^*]$

the probability of finding the particle in the whole space is unity.

$$\int_{\text{all space}} \psi^*\psi\, \mathrm{d}^3\mathbf{r} = 1$$

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continuity equation or the conservation of probability density

$$\nabla \cdot \mathbf{j} + \frac{\partial}{\partial t}\rho = 0$$

The expectation value of any physical quantity is given by

$$\langle O \rangle = \int_V \psi^*(\mathbf{r}, t) O \psi(\mathbf{r}, t)\, d^3\mathbf{r}$$

Position $\quad \mathbf{r}_{op} = \mathbf{r}$

Momentum $\quad \mathbf{p}_{op} = \frac{\hbar}{\mathrm{i}} \nabla$

using the separation of variables:

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r})\, \mathrm{e}^{-\mathrm{i}Et/\hbar}$$

and

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

In general, any solution of the Schrödinger equation may be constructed from the superposition of these stationary solutions:

$$\psi(\mathbf{r}, t) = \sum_n a_n \psi_n(\mathbf{r})\, e^{-iE_n t/\hbar} + \int a_E \psi_E(\mathbf{r})\, e^{-iEt/\hbar}\, dE \qquad (3.1.12)$$

For a two-particle system, we use a wave function $\psi(\mathbf{r}_1, \mathbf{r}_2, t)$ to describe the particle 1 at $\mathbf{r}_1$, and particle 2 at $\mathbf{r}_2$, at time $t$. Here we assume that the two particles are not identical, such as those of a hydrogen atom. The Hamiltonian is

$$H = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + V(\mathbf{r}_1 - \mathbf{r}_2) \qquad (3.1.13)$$

$$\mathbf{p}_1 = \frac{\hbar}{i}\nabla_1$$

$$\mathbf{p}_2 = \frac{\hbar}{i}\nabla_2$$

# THE SQUARE WELL

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V(z)\right]\phi(z)=E\phi(z)$$

## 3.2.1 Infinite Barrier Model

$$\phi_n(z)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}z\right)\qquad n=1,2,3,\ldots$$

with corresponding energy and wave number

$$E_n=\frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2\qquad k_z=\frac{n\pi}{L}$$

If the origin of the coordinate $z=0$ is chosen at the center of the well, $V(+z)=V(-z)$, the solution can always be put in terms of even or odd functions by parity consideration:

$$\phi_n(z)=\begin{cases}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}z\right) & n \text{ even}\\ \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}z\right) & n \text{ odd}\end{cases}\tag{3.2.4}$$

The complete solution for the potential well $V(z)$ in a three-dimensional space is solved from

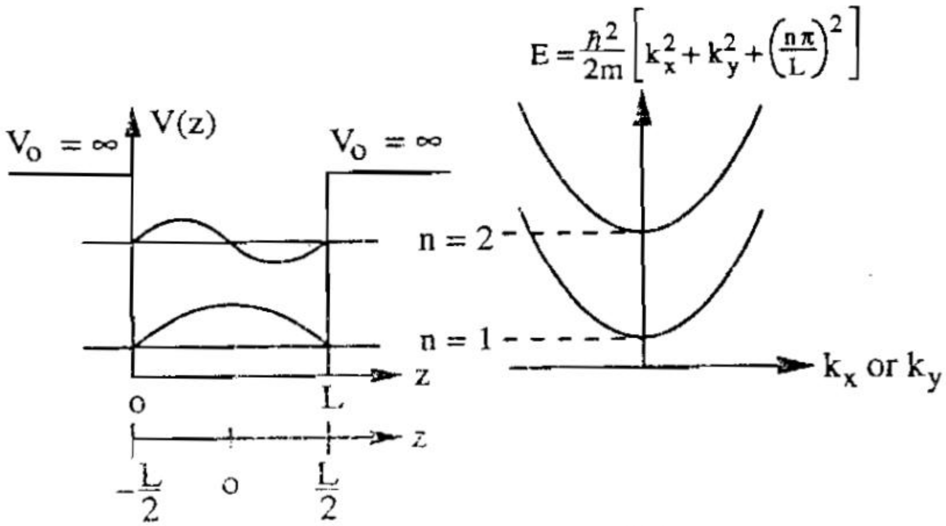
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(z)\right]\psi(x, y, z) = E\psi(x, y, z) \qquad (3.2.7)$$

The normalized wave function is

$$\psi(x, y, z) = \frac{e^{ik_x x + ik_y y}}{\sqrt{A}}\phi_n(z) \qquad (3.2.8)$$

with a corresponding energy

$$E = \frac{\hbar^2}{2m}\left[k_x^2 + k_y^2 + \left(\frac{n\pi}{L}\right)^2\right] \qquad (3.2.9)$$




(a) (b)

For a GaAs/$Al_xGa_{1-x}$As quantum-well structure,

width is 100 Å

$$m_e^* = 0.0665 m_0$$

quantized electron subband energies are

$$E_n = \frac{\hbar^2}{2m_e^*}\left(\frac{n\pi}{L}\right)^2 = n^2 E_1 = E_1, 4E_1, 9E_1, \ldots$$

where

$$E_1 = \frac{\hbar^2}{2m_e^*}\left(\frac{\pi}{L}\right)^2 = \frac{1}{(m_e^*/m_0)L^2} \times 37.6 \text{ eV}$$

$$= \frac{1}{0.0665 \times 100^2} \times 37.6 \text{ eV} = 56.5 \text{ meV}$$

Therefore, we find the subband energies are

$$E_n = 56.5, 226, 508.5, \ldots (\text{meV}$$

# Two-Dimensional Density of States.

$$n = \frac{2}{V}\sum_{n}\sum_{k_x}\sum_{k_y} f(E)$$

*Intergration Form*

$$\frac{2}{V}\sum_{k_x}\sum_{k_y} = \frac{2}{V}\int\frac{\mathrm{d}k_x}{2\pi/L_x}\int\frac{\mathrm{d}k_y}{2\pi/L_y} = \frac{2}{L_z}\int\frac{\mathrm{d}k_x\,\mathrm{d}k_y}{(2\pi)^2}$$

$$= \frac{2}{L_z}\int\frac{2\pi k_t\,\mathrm{d}k_t}{(2\pi)^2} = \frac{m^*}{\pi\hbar^2 L_z}\int_{E_n}^{\infty}\mathrm{d}E$$

$k_t^2 = k_x^2 + k_y^2$, $\mathrm{d}E = \hbar^2 k_t\,\mathrm{d}k_t/m^*$

$$\rho_{2D}(E) = \frac{m^*}{\pi\hbar^2 L_z}\sum_n H(E - E_n)$$ to compare $$\rho_{3D}(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}$$

where $H(x)$ is a Heaviside step function $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x < 0$.

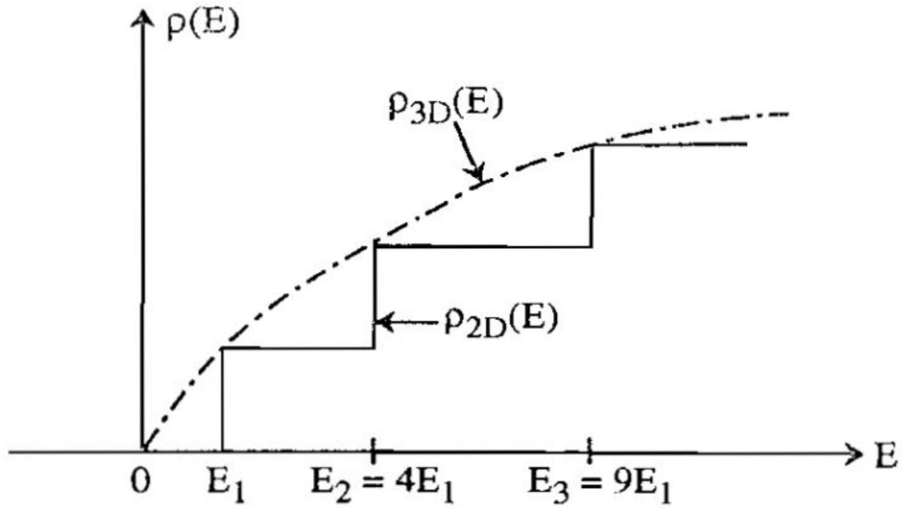



**Figure 3.2.** The electron density of states $\rho_{2D}(E)$ solid line for a two-dimensional quantum-well structure is compared with the three-dimensional density of states $\rho_{3D}(E)$ (dashed curve).

$$n = \int \mathrm{d}E \rho_{2D}(E) f(E)$$

*Example* As a numerical example, we calculate the electron density of states for a bulk GaAs semiconductor at an energy 0.1 eV above the conduction

$$\rho_{3D}(E - E_c = 0.1\ \mathrm{eV}) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(E - E_c)^{1/2}$$
$$= 3.69 \times 10^{19}\ (\mathrm{cm}^{-3}\ \mathrm{eV}^{-1})$$

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For a quantum well with $L_z = 100$ Å, we estimate the density of states of the first step (with $E_1 = 56.5$ meV):

$$\rho_{2D}(E - E_1) = \frac{m_e^*}{\pi \hbar^2 L_z} = 2.78 \times 10^{19}\ (\mathrm{cm}^{-3}\ \mathrm{eV}^{-1})$$

We can also estimate the carrier concentration with an energy spread of $k_B T = 0.026$ eV at 300 K and obtain

$$n \sim 2.78 \times 10^{19} \times 0.026 = 7.2 \times 10^{17}\ \mathrm{cm}^{-3}$$

# One-Dimensional Density of States.

(1D) quantum wire along

$$n = \frac{2}{V} \sum_{n_x, n_y} \sum_{k_z} f(E)$$

$$E = E_{n_x} + E_{n_y} + \frac{\hbar^2}{2m^*}k_z^2$$

$$E_{n_x} = \frac{\hbar^2}{2m^*}\left(\frac{n_x\pi}{L_x}\right)^2 \qquad E_{n_y} = \frac{\hbar^2}{2m^*}\left(\frac{n_y\pi}{L_y}\right)^2$$

$n_x, n_y = 1, 2, 3, \ldots,$ and $k_z$ is a continuous variable. Using

$$\frac{2}{V}\sum_{n_x,n_y}\sum_{k_z} = \frac{2}{L_xL_y}\sum_{n_x,n_y}\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}$$

$$= \frac{1}{\pi L_xL_y}\sqrt{\frac{2m^*}{\hbar^2}}\sum_{n_x,n_y}\int_{E_{n_x}+E_{n_y}}^{\infty}\frac{dE}{\sqrt{E-E_{n_x}-E_{n_y}}}$$

the 1D density of states $\rho_{1D}(E)$ is

$$\rho_{1D}(E) = \frac{1}{\pi L_xL_y}\sqrt{\frac{2m^*}{\hbar^2}}\sum_{n_x,n_y}\frac{1}{\sqrt{E-E_{n_x}-E_{n_y}}} \qquad E > E_{n_x} + E_{n_y}$$

### 3.2.2 Finite Barrier Model

For a finite barrier quantum well, as shown in Fig. 3.3, we have

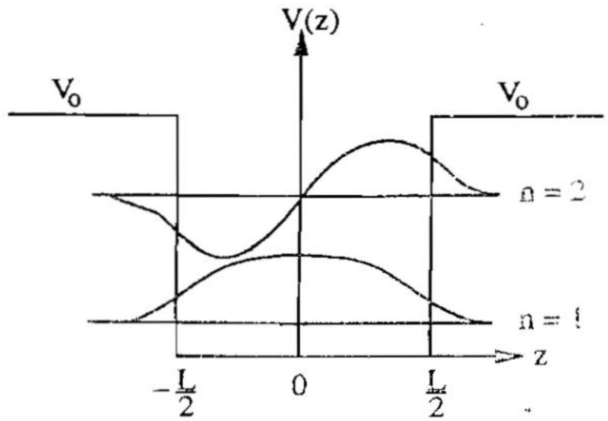
$$V(z) = \begin{cases} V_0 & |z| \geq \frac{L}{2} \\ 0 & |z| < \frac{L}{2} \end{cases}$$

$$\left[ -\frac{d}{dz}\frac{1}{m}\frac{d}{dz} + V(z) \right] \phi(z) = E\,\phi(z)$$

$$\phi(z) = \begin{cases} C_1\, e^{-\alpha(|z| - L/2)} & |z| \geq \frac{L}{2} \\ C_2 \cos kz & |z| < \frac{L}{2} \end{cases}$$

$$k = \frac{\sqrt{2 m_w E}}{\hbar}$$

$$\alpha = \frac{\sqrt{2 m_b (V_0 - E)}}{\hbar}$$




$$\phi\left(\frac{L^+}{2}\right) = \phi\left(\frac{L^-}{2}\right)$$

$$\frac{1}{m_b}\frac{d}{dz}\phi\left(\frac{L^+}{2}\right) = \frac{1}{m_w}\frac{d}{dz}\phi\left(\frac{L^-}{2}\right)$$

$$\phi(z) = \begin{cases} C_1 e^{-\alpha(z-L/2)} & z > \dfrac{L}{2} \\ C_2 \sin kz & |z| \leq \dfrac{L}{2} \\ -C_1 e^{+\alpha(z+L/2)} & z < -\dfrac{L}{2} \end{cases}$$

$$C_1 = C_2 \sin k\frac{L}{2}$$

$$-\frac{\alpha C_1}{m_b} = \frac{k}{m_w} C_2 \cos k\frac{L}{2}$$

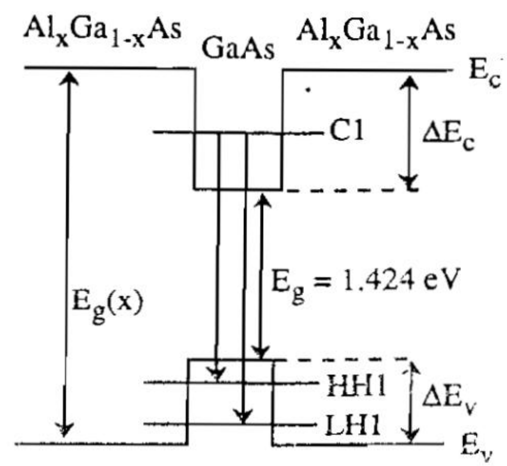
$$\alpha = -\frac{m_b k}{m_w} \cot k\frac{L}{2}$$

**Example** Consider a GaAs/$Al_xGa_{1-x}As$ quantum well shown in Fig. 3.5. Assume the following parameters

$$m_e^* = (0.0665 + 0.0835x)m_0 \qquad m_{hh}^* = (0.34 + 0.42x)m_0$$

$$m_{lh}^* = (0.094 + 0.043x)m_0 \qquad E_g(x) = 1.424 + 1.247x \text{ (eV)}$$

$$(0 \leq x < 0.45, \text{ room temperature})$$



$\Delta E_g(x) = 1.247x$ (eV), $\Delta E_c = 0.67\Delta E_g$, and $\Delta E_v = 0.33\Delta E_g$, where $m_0$ is the free electron mass.



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a. Consider the aluminum mole fraction $x = 0.3$ in the barrier regions ($x = 0$ in the well region) and the well width $L_w = 100$ Å. How many bound states are there in the conduction band? How many bound heavy-hole and light-hole subbands are there?

b. Find the lowest bound-state energies for the conduction subband (C1) and the heavy-hole (HH1) and the light-hole (LH1) subbands for a 100-Å GaAs quantum well in part (a). What are the C1–HH1 and C1–LH1 transition energies?

c. Assume that we define an effective well width $L_{eff}$ using an infinite barrier model such that its ground-state energy is the same as the energy of the first conduction subband $E_{c1}$ in (b). What is $L_{eff}$? If we repeat the same procedure for the HH1 and the LH1 subbands, what are $L_{eff}$?

## SOLUTIONS.

| | $m_e^*$ | $m_{hh}^*$ | $m_{lh}^*$ | $E_g$ |
|---|---|---|---|---|
| Well | $0.0665m_0$ | $0.34m_0$ | $0.094m_0$ | 1.424 eV |
| Barrier ($x = 0.3$) | $0.0916m_0$ | $0.466m_0$ | $0.107m_0$ | 1.798 eV |

$$L_w = 100\ \text{Å},\ \Delta E_c = 0.67\Delta E_g = 0.2506\ \text{eV},\ \Delta E_v = 0.1235\ \text{eV}.$$

a. The number of bound states $N$ is determined by $(N-1)\pi/2 \le \sqrt{2m_w^* V_0}(L/2\hbar) \le N\pi/2$, $V_0 = \Delta E_c$ for electrons and $\Delta E_v$ for holes, respectively.

For electrons: $\sqrt{2m_e^* \Delta E_c}\left(\frac{L}{2\hbar}\right) = 3.30 < N\frac{\pi}{2}$ $\quad N = 3$ bound states

For heavy holes: $\sqrt{2m_{hh}^* \Delta E_v}\left(\frac{L}{2\hbar}\right) = 5.25 < N\frac{\pi}{2}$ $\quad N = 4$ bound states

For light holes: $\sqrt{2m_{lh}^* \Delta E_v}\left(\frac{L}{2\hbar}\right) = 2.76 < N\frac{\pi}{2}$ $\quad N = 2$ bound states

b. The eigenenergy $E$ is found by searching for the root in

$$\alpha = \frac{m_b^*}{m_w} k \tan\left(k\frac{L_w}{2}\right) \qquad \alpha = \sqrt{\frac{2m_b^*(V_0 - E)}{\hbar^2}} \qquad k = \sqrt{\frac{2m_w^* E}{\hbar^2}}$$

For electrons, $m_w^* = 0.0665m_0$, $m_b^* = 0.0916m_0$, and $V_0 = 250.6$ meV,

the first subband energy is

$$E_{C1} = 30.7 \text{ meV}$$

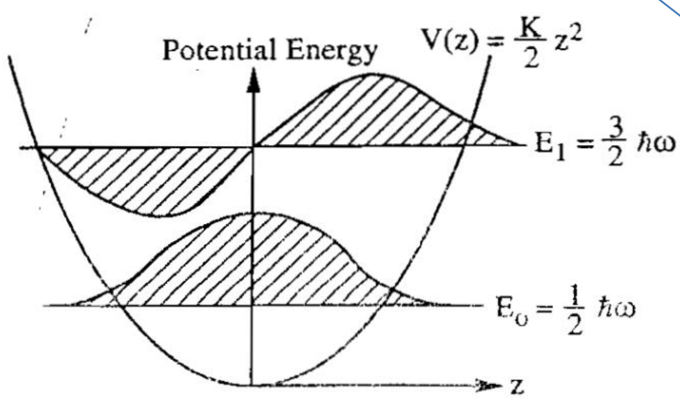
Similarly, $E_{HH1} = 7.4$ meV and $E_{LH1} = 20.6$ meV. The transition energies are

$$E_{C1-HH1} = E_g + E_{C1} + E_{HH1} = 1462 \text{ meV}$$
$$E_{C1-LH1} = E_g + E_{C1} + E_{LH1} = 1475 \text{ meV}$$

# THE HARMONIC OSCILLATOR

$$V(z) = (K/2)z^2$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{K}{2}z^2\right)\phi(z) = E\,\phi(z)$$




If we define

$$\omega = \sqrt{\frac{K}{m}}$$

$$\xi = \alpha z$$

$$\alpha = \sqrt{\frac{m\omega}{\hbar}}$$

$$\left[\frac{d^2}{d\xi^2} + \left(\frac{2E}{\hbar\omega} - \xi^2\right)\right]\phi(\xi) = 0$$

The solutions are the Hermite–Gaussian functions

$$\phi_n(\xi) = \left(\frac{\alpha}{\sqrt{\pi}\,2\pi n!}\right)^{1/2} H_n(\xi)\,e^{-\xi^2/2}$$

where $H_n(\xi)$ are the Hermite polynomials satisfying the differential equation

$$\left(\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + 2n\right)H_n(\xi) = 0 \qquad E = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, 3, \ldots$$

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The first few Hermite polynomials are

$$H_0(\xi) = 1$$
$$H_1(\xi) = 2\xi$$
$$H_2(\xi) = -2 + 4\xi^2$$
$$H_3(\xi) = -12\xi + 8\xi^3$$
$$H_4(\xi) = 12 - 48\xi^2 + 16\xi^4$$

Another elegant way [3] to find the solutions for the harmonic oscillator is to use the matrix approach by defining the annihilation operator

$$a = \sqrt{\frac{m\omega}{2\hbar}}\, z + \frac{ip}{\sqrt{2m\hbar\omega}}$$

and the creation operator

$$a^{+} = \sqrt{\frac{m\omega}{2\hbar}}\, z - \frac{ip}{\sqrt{2m\hbar\omega}}$$

Note the relation

$$zp - pz = i\hbar$$

which can be proved using $p = (\hbar/i)(\partial/\partial z)$ and

$$(zp - pz)\psi = z\frac{\hbar}{i}\frac{\partial}{\partial z}\psi - \frac{\hbar}{i}\frac{\partial}{\partial z}z\psi = i\hbar\psi$$

$$a^+a = \frac{m\omega}{2\hbar}z^2 + \frac{p^2}{2m\hbar\omega} + \frac{i}{2\hbar}(zp - pz)$$
$$= \frac{1}{\hbar\omega}\left(\frac{p^2}{2m} + \frac{m\omega^2}{2}z^2\right) - \frac{1}{2}$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 z^2$$
$$= \hbar\omega\left(a^+a + \frac{1}{2}\right)$$

***Problem is to find the:*** $\boxed{N \equiv a^+a}$

and noting that the Poisson bracket

$$[a, a^+] \equiv aa^+ - a^+a = \frac{i}{2\hbar}\{(pz - zp) - (zp - pz)\} = 1$$
$$Na = a^+aa = (aa^+ - 1)a = aN - a$$
$$Na^+ = a^+aa^+ = a^+(a^+a + 1) = a^+(N + 1)$$

For any eigenstate of $H$ or $N$, say $\phi_n \equiv |n>$

$$\langle n|N|n\rangle = \langle n|a^+a|n\rangle = \langle\psi|\psi\rangle \geq 0$$
$$|\psi\rangle \equiv a|n\rangle$$

$$Na|n\rangle = (aN - a)|n\rangle = (n - 1)a|n\rangle$$

$$a^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$|n\rangle = \frac{(a^{+})^{n}}{\sqrt{n!}}|0\rangle$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2, 3, \ldots$$

$$a|0\rangle = 0$$

$$0 = \langle z|a|0\rangle = \langle z|\sqrt{\frac{m\omega}{2\hbar}}\,z + \sqrt{\frac{\hbar}{2m\omega}}\,\frac{\mathrm{d}}{\mathrm{d}z}|0\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\mathrm{d}}{\mathrm{d}z} + \frac{m\omega}{\hbar}z\right)\phi_0(z)$$

$$\phi_0(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-m\omega z^2/(2\hbar)}$$

# TIME-INDEPENDENT PERTURBATION THEORY

**Perturbation Method**

$$H = H^{(0)} + H'$$

small perturbing

$$H^{(0)}\phi_n^{(0)} = E_n^{(0)}\phi_n^{(0)}$$

$$H\psi = E\psi$$

$$H = H^{(0)} + \lambda H'$$

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots$$

$$\psi = \psi^{(0)} + \lambda \psi^{(1)} + \lambda^2 \psi^{(2)} + \cdots$$

Zeroth order $\quad H^{(0)}\psi^{(0)} = E^{(0)}\psi^{(0)}$

First order $\quad H^{(0)}\psi^{(1)} + H'\psi^{(0)} = E^{(0)}\psi^{(1)} + E^{(1)}\psi^{(0)}$

Second order $\quad H^{(0)}\psi^{(2)} + H'\psi^{(1)} = E^{(0)}\psi^{(2)} + E^{(1)}\psi^{(1)} + E^{(2)}\psi^{(0)}$

**Zeroth-Order Solutions.** It is clearly seen that the zeroth-order solutions are the unperturbed solutions:

$$\psi_n^{(0)} = \phi_n^{(0)} \qquad (3.5.9a)$$

$$E_n^{(0)} = E_n^{(0)} \qquad (3.5.9b)$$

**First-Order Solutions.** The first-order wave function $\psi^{(1)}$ may be expanded in terms of a linear combination of the unperturbed solutions:

$$\psi_n^{(1)} = \sum_m a_{mn}^{(1)} \phi_m^{(0)} \qquad (3.5.10)$$

$$\psi_n = \phi_n^{(0)} + \sum_{m \neq n} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}} \phi_m^{(0)}$$

$$E_n = E_n^{(0)} + H'_{nn}$$

**Second-Order Solutions.** Similarly, the second-order wave function $\psi^{(2)}$ can be expanded in terms of the zero-order solutions:

$$\psi_n^{(2)} = \sum_m a_{mn}^{(2)} \phi_m^{(0)} \tag{3.5.17}$$

We find

$$E_n^{(2)} = \sum_{m \neq n} a_{mn}^{(1)} H'_{nm} = \sum_{m \neq n} \frac{H'_{mn} H'_{nm}}{E_n^{(0)} - E_m^{(0)}} \tag{3.5.18a}$$

and

$$a_{mn}^{(2)} = \sum_{k \neq n} \frac{H'_{mk} H'_{kn}}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_k^{(0)}\right)} - \frac{H'_{mn} H'_{nn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}, \qquad m \neq n \tag{3.5.18b}$$

$$\psi_n = \phi_n^{(0)} + \sum_{m \neq n} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}} \phi_m^{(0)} + \sum_{m \neq n} \left\{ \left[ \sum_{k \neq n} \frac{H'_{mk} H'_{kn}}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_k^{(0)}\right)} - \frac{H'_{mn} H'_{nn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2} \right] \phi_m^{(0)} - \frac{|H'_{mn}|^2}{2\left(E_n^{(0)} - E_m^{(0)}\right)^2} \phi_n^{(0)} \right\} \tag{3.5.21a}$$

$$E_n = E_n^{(0)} + H'_{nn} + \sum_{m \neq n} \frac{|H'_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} \tag{3.5.21b}$$