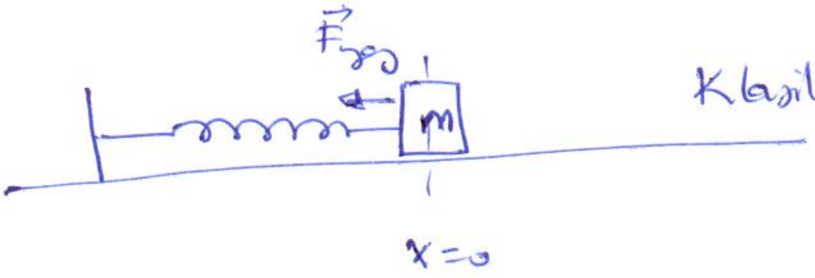
Harmonik Salınıcı (Osilatör)



Klasik bir harmonik salınıcı

$\vec{F}_{ygg} = -kx$ geri çağırıcı kuvvet olmak üzere

m: kütleli cismin hareket denklemi sürtünme yokken

$F = ma$'dan $\quad -kx = m\dfrac{d^2x}{dt^2}$

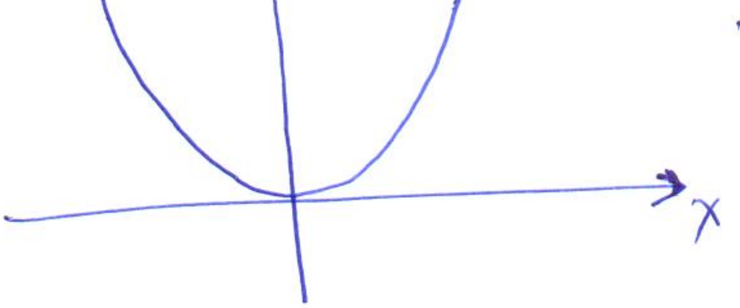
$$\boxed{\frac{d^2x}{dt^2} + \frac{k}{m}x = 0}$$ old. hatırlayalım.

$\omega^2 \equiv \dfrac{k}{m} \rightarrow \omega^2$: birim kütle ve birim uzunluk başına geri çağırıcı kuvvettir.

$\omega = \sqrt{\dfrac{k}{m}} \Rightarrow$ salınıcının açısal frekansı

$\Delta U = -\int F dx$ olduğu hatırlanırsa

$\Delta U = \dfrac{1}{2}kx^2$ bu klasik sistemin potansiyel enerjisidir.



$V(x) = \dfrac{1}{2}kx^2$

Klasik bu sistemi kuantum sistemi olarak çalışalım.

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2}+\frac{1}{2}kx^2u=Eu}$$ olur.

$$\boxed{E=\frac{\hbar\omega}{2}\varepsilon} \quad \text{ve} \quad \boxed{x=\sqrt{\frac{\hbar}{m\omega}}\,y} \quad \text{ve} \quad \boxed{k=m\omega^2}$$

dönüşümlerini uygulayalım.

$$dx=\sqrt{\frac{\hbar}{m\omega}}\,dy \Rightarrow dx^2=\frac{\hbar}{m\omega}dy^2 \text{ olur.}$$

$$-\frac{\hbar^2}{\cancel{2}m}\frac{d^2u}{\frac{\hbar}{m\omega}dy^2}+\frac{1}{\cancel{2}}m\omega^2\frac{\hbar}{m\omega}y^2u=\frac{\hbar\omega}{\cancel{2}}\varepsilon u$$

$$\Rightarrow \boxed{-\hbar\omega\frac{d^2u}{dy^2}+\hbar\omega y^2u=\hbar\omega\,\varepsilon u} \text{ olur}$$

$$\Rightarrow \boxed{\frac{d^2u}{dy^2}+(\varepsilon-y^2)u(y)=0}$$

elde edilir.

<u>Öncelikle:</u> Bu diferansiyel denklemin $y\to\infty$'a giderkenki asimtotik davranışına bakalım. $y\to\infty$ giderken y^2 çok daha hızlı ∞'a gider. Bu durumda

$$y^2 >>> \varepsilon$$ ~~olur~~

olur ve ε $y\to\infty$'da önemsiz kalır. Böylece

$y \to \infty$'a giderken $u(y\to\infty) \equiv u_0(y)$

tanımını yaparsak, ve $y^2 >> \varepsilon$ olduğundan;

$$\boxed{\frac{d^2 u_0}{dy^2} - y^2 u_0 \cong 0}$$

denkleminin çözümleri $y \to \infty$ asimtotik davranışını verecektir.

Bu denklemi

$$\frac{d}{dy}\left[\left(\frac{du_0}{dy}\right)^2 - y^2 u_0^2\right] + 2y u_0^2 \cong 0$$

olarak yazmak da mümkündür.

$$u(y\to\infty) = u_0(y) \to 0 \Rightarrow$$

$[u_0(y)]^2$ çok daha hızlı sıfıra gider.

Böylece;

$$\frac{d}{dy}\left[\left(\frac{du_0}{dy}\right)^2 - y^2 u_0^2\right] \cong 0 \quad \text{denklemiyle}$$

~~ile~~ ilgilenebiliriz. Bu denklem sıfıra eşitse türevin için keyfi bir sabit eşit olacaktır.

$$\left(\frac{du_0}{dy}\right)^2 - y^2 u_0^2 \approx C \qquad C: \text{keyfi sabit}$$

$$\Rightarrow \frac{du_0}{dy} = \pm\sqrt{C + y^2 u_0^2} \quad \text{olur.}$$

Hem u_0 hem de $\frac{du_0}{dy}$ $y \to \infty$'a giderken sıfıra gitmelidir. Bu nedenle $C = 0$ olmalıdır.

Böylece;

$$\frac{du_0}{dy} \cong \pm y\, u_0$$

olur. Denklemin çözümleri

$$u_0(y) = e^{\pm y^2/2}$$

olur. $y \to \pm\infty$ giderken $u_0(y) \to 0$'a gitmelidir. Bu nedenle fiziksel çözüm

$$u_0(y) = e^{-y^2/2}$$

olur. Tekrar asıl denkleme dönelim.

$$u(y) \equiv h(y)\, u_0(y)$$

$$u = h(y)\, e^{-y^2/2}$$

yazabiliriz. Çünkü $y \to \infty$'da davranışı biliyoruz. Önerdiğimiz çözümü;

$$\frac{d^2u}{dy^2} + (\varepsilon - y^2)\, u = 0$$ 'a

uygularsak;

$$\boxed{\frac{d^2h(y)}{dy^2} - 2y\frac{dh(y)}{dy} + (\varepsilon - 1)\, h(y) = 0}$$

denklemine ulaşırız. Bu denklemde H.O'nun $y<\infty$ davranışını inceleyelim.

Bu denklem için

$$h(y) = \sum_{m=0}^{\infty} a_m y^m$$

kuvvet serisi çözümü önerilirse,

$$\frac{dh(y)}{dy} = \sum_{m=0}^{\infty} m a_m y^{m-1} \quad \text{ve}$$

$$\frac{d^2 h(y)}{dy^2} = \sum_{m=0}^{\infty} m(m-1) a_m y^{m-2}$$

olur. Taraflar denklemde yerine konursa,

$$\sum_{m=0}^{\infty} m(m-1) a_m y^{m-2} - 2y \sum_{m=0}^{\infty} m a_m y^{m-1} + (\varepsilon-1) \sum_{m=0}^{\infty} a_m y^m = 0$$

$$\Rightarrow \boxed{\sum_{m=0}^{\infty} m(m-1) a_m y^{m-2} = \sum_{m=0}^{\infty} (2m-\varepsilon+1) a_m y^m}$$

olur. Sol tarafı inceleyelim,

$$\sum_{m=0}^{\infty} m(m-1) a_m y^{m-2} = 0 + 0 + \sum_{m=2}^{\infty} m(m-1) a_m y^{m-2}$$

olur.

$$m \longrightarrow m+2 \text{ geçişi yapılırsa,}$$

$$\sum_{m=0}^{\infty} m(m-1) a_m y^{m-2} \longrightarrow \sum_{m=0}^{\infty} (m+2)(m+1) a_{m+2} y^m$$

olur. Böylece,

$$\sum_{m=0}^{\infty}(m+2)(m+1)a_{m+2}y^m = \sum_{m=0}^{\infty}(2m-\varepsilon+1)a_m y^m$$

sonucuna ulaşılır. Bu eşitlik;

$$(m+2)(m+1)a_{m+2} = (2m-\varepsilon+1)a_m$$

olursa sağlanır. Bu durumda

$$\boxed{a_{m+2} = \frac{2m-\varepsilon+1}{(m+2)(m+1)}a_m}$$

kat sayılar denklemine ulaşılır.

Eğer; a_0 biliniyorsa

$a_2, a_4, a_6, \ldots \quad , m=2,4,6\ldots$

a_1 biliniyorsa

$a_3, a_5, a_7, \ldots \quad , m=3,5,7,\ldots$

kat sayıları hesaplanabilir.

$m=0 \qquad a_2 = \dfrac{1-\varepsilon}{2.1}a_0$

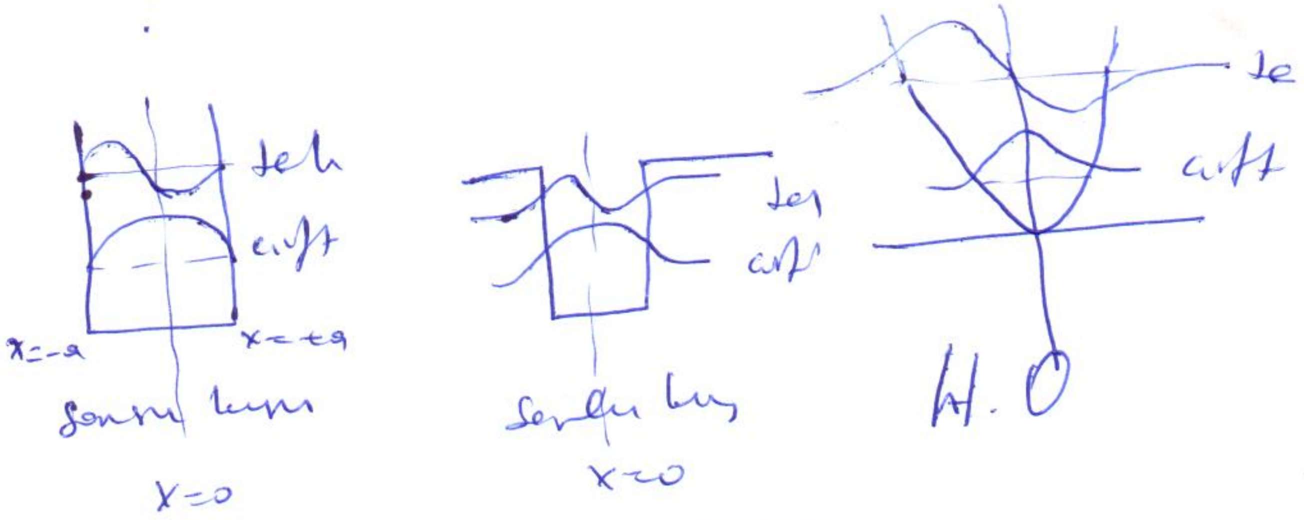
$m=2 \qquad a_4 = \dfrac{5-\varepsilon}{4.3}a_2 = \dfrac{(5-\varepsilon)(1-\varepsilon)}{4.3.2.1}a_0$

$\vdots$

$$m=1 \Rightarrow a_3 = \frac{(3-\varepsilon)}{3.2} a_1$$

$$m=2 \Rightarrow a_5 = \frac{(7-\varepsilon)}{5.4} a_3 = \frac{(7-\varepsilon)(3-\varepsilon)}{4.4.3.2} a_1$$

$\vdots$



m'nin çok büyük değerleri için;

$$\boxed{m > N \quad N: \text{çok büyük sayı}}$$

$$a_{m+2} = \frac{m\left(2 - \frac{\varepsilon}{m} + \frac{1}{m}\right)}{m^2\left(1+\frac{2}{m}\right)\left(1+\frac{1}{m}\right)} a_m \Rightarrow$$

$$\boxed{a_{m+2} \approx \frac{2}{m} a_m}$$

olur. $h(y)$ 'nin çift fonksiyon halini yani dif. denk. çift çözümlerini incelersek;

$$m = N \Rightarrow a_{N+2} = \frac{2}{N} a_N$$

$$m = N+2 \Rightarrow a_{N+4} = \frac{2}{N+2} a_{N+2} = \frac{2}{(N+2)N} a_N$$

$$\vdots$$

olarak devam eder. Bu durumda

$$h(y) = \sum_{m=0}^{\infty} a_m y^m = \left(\begin{matrix} m<N \text{ dereceli bir} \\ \text{polinom} \end{matrix} \right)$$

$$+ a_N \left[y^N + \frac{2}{N} y^{N+2} + \frac{2^2}{N(N+2)} y^{N+4} + \dots \right]$$

olur. $m > N$ serisi

$$a_N y^2 \left(\frac{N}{2}-1\right)! \left[\frac{(y^2)^{\frac{N}{2}-1}}{(N/2-1)!} + \frac{(y^2)^{N/2}}{(N/2)!} + \dots \right]$$

olarak yazılabilir. $\boxed{N=2k}$ seçilirse

böylece tek çözümlerde $N=2k+1$ ile ifade edilebilir.

$$y^2 (k-1)! \left[\frac{(y^2)^{k-1}}{(k-1)!} + \frac{(y^2)^k}{k!} + \dots \right]$$

$$= y^2 (k-1)! \left[e^{y^2} - \left\{ 1 + y^2 + \frac{(y^2)^2}{2!} + \dots \right\} \right]$$

olur.

$u(y) = h(y) e^{-y^2/2}$ olduğu hatırlanırsa.

$h(y)$'nin içindeki "e^{y^2}" terimlerden

dolayı; $u(y) \propto e^{y^2} e^{-y^2/2} = e^{y^2/2}$

orantılılığı ortaya çıkar. Buna göre

$$u(y \to \infty) \to 0$$

olamaz. Kabul edilebilir bir

çözüm için

$$h(y) = \sum_{m=0}^{\infty} a_m y^m$$

serisini sonlandıracak bir şart lazımdır.

Eğer;

$$\varepsilon = 2n+1$$

seçilirse a_m'leri sonlu sayıda tutacak

şart ortaya konmuş olur. Böylece;

çift $$a_{2k} = (-2)^k \frac{n(n-2)\ldots(n-2k+4)(n-2k+2)}{(2k)!} a_0$$

tek $$a_{2k+1} = (-2)^k \frac{(n-1)(n-3)\ldots(n-2k+3)(n-2k+1)}{(2k+1)!} a_1$$

çözümleri elde edilir.

Böylece;

(1) $\varepsilon = 2n+1$ ve $E = \frac{\hbar\omega}{2}\varepsilon \Rightarrow \boxed{E_n = \hbar\omega(n+\frac{1}{2})}$

$n = 0, 1, 2, 3, \ldots$

eşit aralıklı ~~....~~ kesikli
enerji öz değerleri elde edilmiş olur.

$$E_{n+1} - E_n = \hbar\omega$$

(2) $h(y)$ aslında normalize edilmemiş
bir hermite polinomudur.

$H_n(y) \equiv$ Hermite polinomları,

$$\frac{d^2 H_n}{dy^2} - 2y\frac{dH_n}{dy} + 2nH_n = 0$$

diff. denkleminin çözümleridir.

where, for simplicity, we have only taken the even solution. The series may be written in the form

$$a_N y^2\left(\frac{N}{2}-1\right)!\left[\frac{(y^2)^{N/2-1}}{(N/2-1)!}+\frac{(y^2)^{N/2}}{(N/2)!}+\frac{(y^2)^{N/2+1}}{(N/2+1)!}+\cdots\right]$$

If we choose $N = 2k$ for convenience, the series takes the form

$$y^2(k-1)!\left[\frac{(y^2)^{k-1}}{(k-1)!}+\frac{(y^2)^{k}}{k!}+\frac{(y^2)^{k+1}}{(k+1)!}+\cdots\right]$$

$$= y^2(k-1)!\left[e^{y^2}-\left\{1+y^2+\frac{(y^2)^2}{2!}+\cdots+\frac{(y^2)^{k-2}}{(K-2)!}\right\}\right]$$

which is of the form of a polynomial + a constant $\times\ y^2e^{y^2}$. When this is inserted into (4-98), we get a solution that does not vanish at infinity. An acceptable solution can be found if the recursion relation (4-101) terminates—that is, if

$$\varepsilon = 2n + 1 \tag{4-103}$$

For that particular value of ε the recursion relations yield

$$a_{2k} = (-2)^k\frac{n(n-2)\cdots(n-2k+4)(n-2k+2)}{(2k)!}a_0 \tag{4-104}$$

and

$$a_{2k+1} = (-2)^k\frac{(n-1)(n-3)\cdots(n-2k+3)(n-2k+1)}{(2k+1)!}a_1 \tag{4-105}$$

Thus the results are:

1. There are discrete, equally spaced eigenvalues. Equation (4-103) translates into

$$E = \hbar\omega(n+\tfrac{1}{2});\ n = 0, 1, 2, \ldots \tag{4-106}$$

a form that looks familiar, since the relation between energy and frequency is the same as that discovered by Planck for the radiation field modes. This is no accident, since a decomposition of the electromagnetic field into normal modes is essentially a decomposition into harmonic oscillators that are decoupled.

2. The polynomials $h(y)$ are, except for normalization constants, the Hermite polynomials $H_n(y)$, whose properties can be found in any number of textbooks on mathematical physics. We limit ourselves to the following outline of their properties:

$H_n(y)$ satisfy the differential equation

$$\frac{d^2H_n(y)}{dy} - 2y\frac{dH_n(y)}{dy} + 2nH_n(y) = 0 \tag{4-107}$$

They satisfy the following recursion relations

$$H_{n+1} - 2yH_n + 2nH_{n-1} = 0 \tag{4-108}$$

$$H_{n+1} + \frac{dH_n}{dy} - 2yH_n = 0 \tag{4-109}$$

Also,

$$\sum_n H_n(y)\frac{z^n}{n!} = e^{2zy-z^2} \tag{4-110}$$

or, equivalently,

$$\frac{d}{dy}\left[\left(\frac{du_0}{dy}\right)^2 - y^2u_0^2\right] = -2yu_0^2 \tag{4-93}$$

This simplifies a great deal if we neglect the term on the right side of the equation. We assume that this can be done, and then check that the assumption was correct. If we drop the right side, we find that

$$\frac{du_0}{dy} = (C + y^2u_0^2)^{1/2} \tag{4-94}$$

where C is a constant of integration. Since both $u_0(y)$ and du_0/dy must vanish at infinity, we must have $C = 0$. Thus

$$\frac{du_0}{dy} = \pm yu_0 \tag{4-95}$$

whose solution, acceptable at infinity, is

$$u_0(y) = e^{-y^2/2} \tag{4-96}$$

We can now check that $2yu_0^2 = 2y\, e^{-y^2}$ is indeed negligible compared with

$$\frac{d}{dy}(y^2u_0^2) = \frac{d}{dy}(y^2 e^{-y^2}) \simeq -2y^3 e^{-y^2} \tag{4-97}$$

for large y. If we now introduce a new function $h(y)$, such that

$$u(y) = h(y)e^{-y^2/2} \tag{4-98}$$

then the differential equation is easily seen to take the form

$$\frac{d^2h(y)}{dy^2} - 2y\frac{dh(y)}{dy} + (\varepsilon - 1)\, h(y) = 0 \tag{4-99}$$

This may not seem like much of a simplification, but we have accounted for the behavior at infinity, and we can now look at the behavior near $y = 0$. Let us attempt a power series expansion

$$h(y) = \sum_{m=0}^{\infty} a_m y^m \tag{4-100}$$

When this is inserted into the equation, we find that the coefficients of y^m satisfy the recursion relation

$$(m + 1)(m + 2)\, a_{m+2} = (2m - \varepsilon + 1)\, a_m \tag{4-101}$$

Thus, given a_0 and a_1, the even and odd series can be generated separately. That they do not mix is a consequence of the invariance of the Hamiltonian under reflections. For arbitrary ε, we find that for large m (say, $m > N$)

$$a_{m+2} \simeq \frac{2}{m}\, a_m \tag{4-102}$$

This means that the solution is approximately

$$h(y) = (\text{a polynomial in } y) + a_N\left[y^N + \frac{2}{N}y^{N+2} + \frac{2^2}{N(N+2)}y^{N+4} + \frac{2^3}{N(N+2)(N+4)}y^{N+6} + \cdots\right]$$

and

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2} \tag{9-111}$$

The normalization of the Hermite polynomials is such that

$$\int_{-\infty}^{\infty} dy\, e^{-y^2} H_n(y)^2 = 2^n n! \sqrt{\pi} \tag{4-112}$$

We list a few of the Hermite polynomials here:

$$\begin{aligned}
H_0(y) &= 1 \\
H_1(y) &= 2y \\
H_2(y) &= 4y^2 - 2 \\
H_3(y) &= 8y^3 - 12y \\
H_4(y) &= 16y^4 - 48y^2 + 12 \\
H_5(y) &= 32y^5 - 160y^3 + 120y
\end{aligned}$$

The orthogonality of eigenfunctions corresponding to different values of n is easily established. The eigenvalue equations

$$\frac{d^2 u_n}{dx^2} = \frac{mk}{\hbar^2} x^2 u_n - \frac{2mE_n}{\hbar^2} u_n$$

and

$$\frac{d^2 u_l^*}{dx^2} = \frac{mk}{\hbar^2} x^2 u_l^* - \frac{2mE_l}{\hbar^2} u_l^*$$

when multiplied by u_l^* and u_n, respectively, and the second equation is subtracted from the first one, yields

$$\frac{d}{dx}\left(u_l^* \frac{du_n}{dx} - \frac{du_l^*}{dx} u_n\right) = \frac{2m}{\hbar^2} (E_l - E_n)\, u_l^* u_n$$

When this equation is integrated over x from $-\infty$ to $+\infty$, the left-hand side vanishes, since the eigenfunctions and their derivatives vanish at $x = \pm\infty$. Thus

$$(E_l - E_n) \int_{-\infty}^{\infty} dx\, u_l^*(x) u_n(x) = 0 \tag{4-114}$$

which means that the eigenfunctions for which $E_l \neq E_n$ are orthogonal. The reason for the importance of the harmonic oscillator in quantum mechanics, as in classical mechanics, is that any small perturbation of a system from its equilibrium state will give rise to small oscillations, which are ultimately decomposable into normal modes—that is, independent oscillators.

3. As (4-106) shows, even the lowest state has some energy, the *zero-point energy*. Its presence is a purely quantum mechanical effect, and can be interpreted in terms of the uncertainty principle. It is the zero-point energy that is responsible for the fact that helium does not "freeze" at extremely low temperatures, but remains liquid down to temperatures of the order of 10^{-3} K, at normal pressures. The fre-

quency ω is larger for lighter atoms, which is why the effect is not seen for nitrogen, say. It also depends on detailed features of the interatomic forces, which is why liquid hydrogen does freeze.

Figure 4-18 shows the shapes of the lowest six eigenfunctions.

Another class of one-dimensional potentials of physical interest are periodic potentials, which satisfy the condition

$$V(x) = V(x + a)$$

Such potentials lead to *band structure* in the energy spectrum—that is, continuous values of allowed energies separated by gaps. This is a rather space- and time-consuming project, and we leave it to Supplement 4-C **[www.wiley.com/college/gasiorowicz]**.

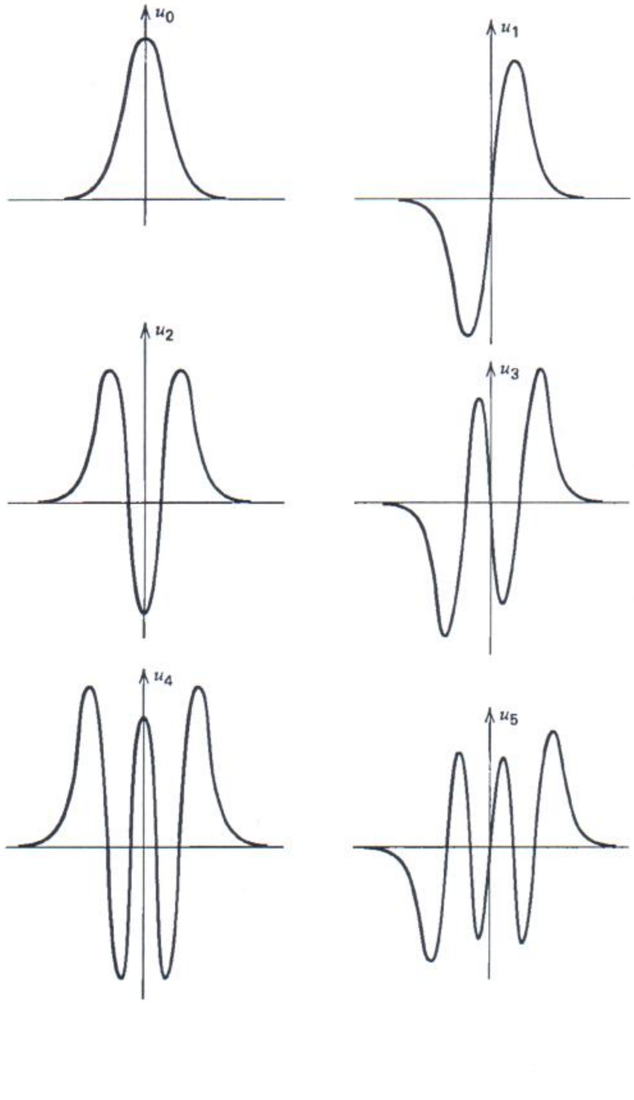


Figure 4-18 The shapes of the first six eigenfunctions.