21 Orthogonal Polynomials

We can construct a polynomial orthonormal basis of a Hilbert space. They are called orthogonal polynomials, which have a beautiful general theory and many important numerical applications ($\rightarrow$**22**).

Key words: generalized Fourier expansion, generalized Rodrigues' formula, generating function, three term recursion relation, zeros, Sturm's theorem, Legendre polynomial, Hermite polynomial, Chebychev polynomial

Summary:
(1) Recognize that there is a set of relations and formulas common to many (all classical) orthogonal polynomials (**21A.3-11**).
(2) Generating function is a useful tool to derive recursion relations (**21B.4**, for example).
(3) Remember where the representative polynomials – Legendre, Hermite, and Chebychev – appear (**21B**).

21.A General Theory

21A.1 Existence of general theory. The most important fact about orthonormal polynomials is that there is a general theory shared by all the families of (classical $\rightarrow$**21A.6** Discussion (A)) orthogonal polynomials. The general theory includes generalized Rodrigues' formula, associating (Sturm-Liouville type) eigenvalue problems, generating functions, three term recursion formulas, etc.

21A.2 Orthogonal polynomials for $L_2([a,b],w)$ via Gram-Schmidt. $\{1, x, x^2, \cdots\}$ makes a complete set of functions for $L_2([a,b],w)$ ($\rightarrow$**20.19**): notice first that $C^0([a,b])$ (the totality of continuous functions on $[a,b]$) is dense in this space. Weierstrass' theorem ($\rightarrow$**17.3**) tells us that any continuous function on a finite interval can be uniformly approximated by a polynomial. Hence, the totality of polynomials is dense in $L_2([a,b],w)$. Therefore, the set of kets $\{|n\rangle\}$ such that $\langle x|n\rangle = x^n$[308] is

[308]For the notational convention see **20.21**.

a complete set ($\to$**20.3**) of the Hilbert space $L_2([a,b],w)$. In this space the scalar product ($\to$**20.5**) is defined by

$$\langle f|g\rangle \equiv \int_a^b \overline{f(x)}g(x)w(x)dx, \tag{21.1}$$

and the norm $\|f\|_w \equiv \sqrt{\langle f|f\rangle}$. We apply the Gram-Schmidt orthonormalization ($\to$**20.16**) to $\{|n\rangle\}$ as follows:
(1) We define $|p_0\rangle = |0\rangle/\sqrt{\langle 0|0\rangle}$.
(2) Normalizing $|1\rangle - |p_0\rangle\langle p_0|1\rangle$, we construct $|p_1\rangle$.
(3) More generally, normalizing

$$|n\rangle - \sum_{k=0}^{n-1} |p_k\rangle\langle p_k|n\rangle, \tag{21.2}$$

we obtain $|p_n\rangle$.
$\{|p_n\rangle\}$ is an orthonormal basis of $L_2([a,b],w)$.

The family of orthogonal polynomials of $L_2([a,b],w)$ is defined by $\langle x|p_n\rangle$ times appropriate n-dependent numerical multiplicative factor as seen in **21A.5**.

Exercise.
Apply the Gram-Schmidt orthonormalization method to $\{x^n\}_{n=0}^{\infty}$ and make an ON basis for $L_2([0,1])$. Compute the basis up to the third member of the set.

21A.3 Theorem.

(1) $p_n(x) = \langle x|p_n\rangle$ is orthogonal to any $(n-1)$-order polynomial.
(2) The orthonormal polynomials for $L_2([a,b],w)$ are unique, if the coefficients of the highest order terms are chosen to be positive.[309]
These assertions are obviously true by construction, but practically important.

21A.4 Least square approximation and generalized Fourier expansion. Let $\mathcal{P}_n$ be the totality of the polynomials order less than or equal to n. The polynomial $P \in \mathcal{P}_n$ which minimizes

$$\|f - P\|_w \tag{21.3}$$

for $f \in L_2([a,b],w)$ is called the n-th order *least square approximation* of f ($\to$**20.13**). The ket $|P\rangle$ satisfying this condition is given by

$$|P\rangle = \sum_{j=0}^{n} |p_j\rangle\langle p_j|f\rangle, \tag{21.4}$$

[309] Here, it is not meant that the orthonormal basis in terms of polynomials is unique (of course, not). If we demand that there are no two polynomials of the same order in the basis, the choice is unique.

where $|p_i\rangle$ are calculated in **21A.2** with respect to w. That is, $|P\rangle$ is the n-th partial sum of the following generalized Fourier expansion ($\to$**20.14**) of $|f\rangle$

$$|f\rangle = \sum_{j=0}^{\infty} |p_j\rangle\langle p_j|f\rangle. \tag{21.5}$$

Notice that all the general properties of the Fourier series **17.5** apply here as well.

Exercise.
(1) Consider the step function $\langle x|a\rangle = \Theta(x-a)$ on $[-1,1]$ ($a \in (-1,1)$). Expand this in terms of Legendre polynomials ($\to$**21A.5**).

$$\langle p_n|a\rangle = \sqrt{\frac{1}{2(2n+1)}}(P_{n-1}(a) - P_{n+1}(a)). \tag{21.6}$$

$\langle p_0|a\rangle = (1-a)/\sqrt{2}$ as easily seen. Hence,

$$\Theta(x-a) = \frac{1}{2}(1-a) + \frac{1}{2}\sum_{n=1}^{\infty}[P_{n-1}(a) - P_{n+1}(a)]P_n(x). \tag{21.7}$$

(2) Expand x^5 into the generalized Fourier series in terms of Legendre polynomials.

21A.5 Example: Legendre polynomials. A family of orthogonal polynomials of $L_2([-1,1])$ called the Legendre polynomials is defined as

$$P_n(x) = \sqrt{\frac{2}{2n+1}}\langle x|p_n\rangle \tag{21.8}$$

in terms of orthonormal kets $\{|p_n\rangle\}$ constructed for $a=-1$, $b=1$ and $w=1$ in **21A.2**. The coefficient $\sqrt{2/(2n+1)}$ is the multiplicative factor mentioned in **21A.2**. $P_n(x)$ is called the n-th order *Legendre polynomial.* According to our notational rule ($\to$**20.22**)

$$\langle p_n|f\rangle = \int_{-1}^{1} dx\sqrt{\frac{2n+1}{2}}P_n(x)f(x). \tag{21.9}$$

Hence, the corresponding generalized Fourier expansion (21.5) in terms of the Legendre polynomials reads

$$f(x) = \sum_{n=0}^{\infty}\frac{2n+1}{2}P_n(x)\left[\int_{-1}^{1} dxP_n(x)f(x)\right]. \tag{21.10}$$

21A.6 Generalized Rodrigues' formula. Let $F_n(x)$ be defined on $(a,b) \subset \boldsymbol{R}$ as

$$F_n(x) = w(x)^{-1}\frac{d^n}{dx^n}[w(x)s(x)^n], \tag{21.11}$$

where w and s are chosen as

a	b	$w(x)$	$s(x)$
a	b	$(b-x)^\alpha(x-a)^\beta$ $\alpha,\beta>-1$	$(b-x)(x-a)$
a	$+\infty$	$e^{-x}(x-a)^\beta$ $\beta>-1$	$x-a$
$-\infty$	$+\infty$	e^{-x^2}	1

As can easily be seen F_n is an n-th order polynomial (→**2A.1** Exercise (D)). $\{F_n(x)\}$ is a orthogonal polynomial system for $L_2((a,b),w)$ (→**20.17**),[310] because

$$\int_a^b dx\, w(x)F_n(x)F_m(x) = 0 \text{ for } n \neq m. \tag{21.12}$$

(Demonstrate this.) If the interval (a,b) and the weight function w are given, the orthogonal polynomial set[311] is uniquely fixed as seen from the Gram-Schmidt construction (up to multiplicative constants) (→**21A.2**).

For example, with $w=1$ (that is, $\alpha=\beta=0$), $a=-1$ and $b=1$, F_n must (→**21A.3**) be proportional to the Legendre polynomial P_n. Indeed, from (21.11)

$$P_n(x) = \frac{(-2)^{-n}}{n!}F_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n. \tag{21.13}$$

This is called *Rodrigues' formula.*

With a suitable n-dependent numerical coefficient K_n a set of orthogonal polynomials $\{f_n\}$ is defined by

$$f_n(x) = \frac{1}{K_n w(x)}\frac{d^n}{dx^n}[w(x)s(x)^n] \tag{21.14}$$

which is called the *generalized Rodrigues formula* (→**21B.1**).[312]

Discussion.

(A) **Classical polynomials**. The generalized Rodrigues' formula can be introduced in a slightly more abstract fashion as follows:
Consider

$$F_n(x) = w(x)^{-1}\frac{d^n}{dx^n}[w(x)s(x)^n], \tag{21.15}$$

where the following conditions are required:
(1) $F_1(x)$ is a first order polynomial.

[310] If a and b are finite, then $L_2((a,b),w) = L_2([a,b],w)$.
[311] We assume that the polynomials are ordered according to their order (→**20.19**).
[312] Not all the orthogonal polynomials can be obtained from the formula; only the so-called *classical polynomials.*

(2) $s(x)$ is a polynomial in x of degree less than or equal to 2 with real roots.
(3) $w(x)$ is real, positive and integrable on $[a, b]$ and satisfies the boundary conditions $w(a)s(a) = w(b)s(b) = 0$.
It turns out that (i)-(iii) implies that we can only have the cases in the table in **22A.6** (apart from trivial linear transformations, and multiplicative constants).[313]
These polynomials are called *classical polynomials.*
(B) Demonstrate with the aid of Rolle's theorem that all the zeros of $P_n(x)$ are in $[-1, 1]$.

21A.7 Relation to the Sturm-Liouville problem. $f_n(x)$ defined by (21.14) obeys the following equation generally called the Sturm-Liouville equation (→**15.4**, **35.1**)

$$-\frac{d}{dx}\left(w(x)s(x)\frac{d}{dx}f_n(x)\right) = \lambda w(x)f_n(x), \tag{21.16}$$

where λ is a pure number given by

$$\lambda = -n\left(K_1\frac{df_1(0)}{dx} + \frac{n-1}{2}\frac{d^2s(x)}{dx^2}\right). \tag{21.17}$$

This can be demonstrated by a tedious but straightforward calculation. See **35.3** Discussion.

21A.8 Generating functions. In general, the following power series of ζ is called the *generating function* of the orthogonal polynomial set $\{p_n(x)\}$

$$Q(\zeta, x) = \sum_{n=0}^{\infty} A_n p_n(x)\zeta^n, \tag{21.18}$$

where A_n is a numerical constant introduced to streamline the formula. That there is such a function for any orthogonal polynomial family can be seen from the rewriting of generalized Rodrigues' formula (21.11). Using Cauchy's theorem (→**6.14**), we have

$$f_n(z) = \frac{1}{K_n w(z)}\oint_{\partial D} dt \frac{n!}{2\pi i(t-z)^{n+1}} w(t)s(t)^n, \tag{21.19}$$

where $D \subset \boldsymbol{C}$ is a small disk centered at z. We define a new variable ζ as

$$\frac{1}{\zeta} = a\frac{s(t)}{t-z}, \tag{21.20}$$

[313] See P Dennery and A Krzywicki, *Mathematics for Physicists* (Harper and Row, 1967), Section 10.3.

where a is a numerical factor introduced to streamline the final outcome. In terms of this variable (21.19) can be rewritten generally as

$$f_n(z) = \frac{a^n n!}{2\pi i K_n w(z)} \oint_{\partial D'} d\zeta \frac{1}{\zeta^{n+1}} Q(\zeta, z), \tag{21.21}$$

where Q is an appropriate function resulted from the intergrand in (21.19) through the change of variables. This implies

$$Q(\zeta, z) = \sum_{n=0}^{\infty} f_n(z) \frac{K_n w(z) \zeta^n}{a^n n!}. \tag{21.22}$$

21A.9 Generating function for Legendre polynomials. For example, for the Legendre polynomials, $K_n = (-2)^n n!$ and $w(x) = 1$. (21.19) reads (or directly from (21.13))

$$P_n(z) = \frac{1}{2\pi i} \oint_{\partial D} \frac{(t^2-1)^n}{[2(t-z)]^n} \frac{dt}{t-z}, \tag{21.23}$$

which is called *Schläfli's integral.* We choose $a = -1/2$ in (21.21) to get

$$P_n(z) = \frac{1}{2\pi i} \oint_{\partial D'} \frac{1}{\zeta^{n+1}} \frac{d\zeta}{\sqrt{1 - 2z\zeta + \zeta^2}}, \tag{21.24}$$

so that ($\rightarrow$**8B.3(i)**)

$$w(z, \zeta) = \frac{1}{\sqrt{1 - 2z\zeta + \zeta^2}} = \sum_{n=0}^{\infty} P_n(z) \zeta^n. \tag{21.25}$$

This is the generating function for the Legendre polynomials.

Exercise.
Derive (21.24). Use the new variable (following (21.20)) ζ as

$$\frac{1}{\zeta} = \frac{t^2 - 1}{2(t-z)}. \tag{21.26}$$

[Hint. When the reader solves for t, she must choose the correct branch so that $t \to z$ corresponds to $\zeta \to 0$.]

21A.10 Three term recursion formula. Let $\{|p_n\rangle\}$ be a complete set of orthonormal polynomial kets, and k_n be the highest order coefficient of the polynomial $p_n(x) = \langle x|p_n\rangle$. Define

$$\gamma_n = k_{n+1}/k_n, \quad \beta_n = \gamma_n/\gamma_{n-1}, \quad \alpha_n = \gamma_n \langle p_n|x|p_n\rangle. \tag{21.27}$$

Then,

$$p_{n+1}(x) = (\gamma_n x - \alpha_n)p_n(x) - \beta_n p_{n-1}(x). \tag{21.28}$$

this follows easily from (1) of **21A.3**.

Discussion.
Let us demonstrate the assertion.

$$\langle x| \left(|p_n\rangle - x\frac{k_n}{k_{n-1}}|p_{n-1}\rangle \right) \tag{21.29}$$

is a polynomial of degree at most $n-1$. Therefore, it can be expressed as a sum of $\{p_{n-1}, \cdots, p_0\}$.
(1) Demonstrate, because of **21A.3**, that only p_{n-2} and p_{n-1} are needed to express $p_n - xk_n p_{n-1}/k_{n_1}$. Already we have the form of (21.24). [Hint. What happens if there are other remaining terms?]
(2) Determine the coefficients.

21A.11 Zeros of orthogonal polynomials. Let $\{|p_n\rangle\}$ be the orthogonal polynomial kets of $L_2([a,b],w)$ (→**20.19**). Then
(1) All the zeros of $p_n(x) = \langle x|p_n\rangle$ are in the interval (a,b). This is practically very important (→**22A.3**). For a proof see **35.3** Discussion.
(2) All the zeros of $p_n(x)$ are single and the zeros of $p_{n+1}(x)$ are separated by those of $p_n(x)$.

Discussion.
The three term recurrence relation can be written as

$$x\boldsymbol{P}(x) = A\boldsymbol{P}(x) + \boldsymbol{q}(x), \tag{21.30}$$

where $\boldsymbol{P} = (p_0, p_1, \cdots, p_{n-1})^T$, A is a symmetric matrix, and $\boldsymbol{q} = (0, \cdots, 0, k_{n-1}p_n/k_n)$. Choose x to be a zero x_i of p_n, then we have

$$x_i\boldsymbol{P}(x_i) = A\boldsymbol{P}(x_i) \tag{21.31}$$

That is, the zeros of p_n must be the eigenvalues of A, so that they must be real.

21A.12 Remark: how to locate real zeros of polynomials. Drawing graphs with the aid of Mathematica and zooming into the relevant portion of the graphs may be the most practical method. Analytically, there is a famous
Theorem [Sturm]. Assume that the n-th order polynomial P does not have any multiple zero. Let $p_0 \equiv P$ and $p_1 \equiv P'$. Using the theorem of division algorithm, construct p_n as follows:

$$p_{i+1} = p_i q_i - p_{i-1} \quad (i = 1, 2, \cdots, n-1). \tag{21.32}$$

Let $V(c)$ be the number of changes of sign in the sequence $p_0(c), p_1(c), \cdots, p_n(c)$.[314] The number of zeros in the interval $[a,b]$ is given by $V(a) - V(b)$.□

[314]Remove $p_i(c)$ if it is zero from the sequence.

21A.13 Example of Sturm's theorem. Let us study $f(x) = x(x^2 - 1)$. We trivially know that $0, \pm 1$ are the real zeros. First we construct p_i in the theorem as follows:

$$p_0 = x(x^2 - 1);\ p_1 = 3x^2 - 1;\ p_2 = 2x/3;\ p_3 = 1. \tag{21.33}$$

Therefore, we can make, for example, the following table exhibiting the signs and V.

a	p_0	p_1	p_2	p_3	$V(a)$
$+\infty$	+	+	+	+	0
2	+	+	+	+	0
1/2	−	−	+	+	1
−1/2	+	−	−	+	2
$-\infty$	−	+	−	+	3

For example, $V(-1/2) - V(2) = 2$, so there must be two zeros in $(-1/2, 2)$.

Discussion.
Find the number of positive real roots of the following polynomials.
(1) $P(x) = 3x^4 + 2x^2 - x - 5$,
(2) $P(x) = 13x^{21} + 3x^3 - 2$,
(3) (Runge's example)
$P(x) = 3.22x^6 + 4.12x^4 + 3.11x^3 - 7.25x^2 + 1.88x - 7.84$.

21A.14 Descartes' sign rule. Let

$$P(x) = a_0x^n + a_1x^{n-1} + \cdots + a_n \tag{21.34}$$

be a real coefficient polynomial. Let W be the number of the sign change in the sequence $a_0, a_1, \cdots, a_n$ (remove 0 from this sequence before counting). Then the number of strictly positive roots of $P(x) = 0$ is given by W or W minus some even positive number. (Hence, if $W = 1$, that is the answer.)

21.B Representative Examples

21B.1 Table of orthogonal polynomials. ($\rightarrow$**2A.1** Exercise (D)) **21A.6** tells us that various orthogonal polynomial families can be obtained by choosing w and s appropriately and also by choosing appropriate multiplicative numerical factors K_n. Some common examples are given as follows.

name	symbol	domain	$w(x)$	$s(x)$	K_n^{-1}
Legendre	P_n	$[-1,1]$	1	$1-x^2$	$(-1)^n 2^n n!$
Chebychev	T_n	$[-1,1]$	$1/\sqrt{1-x^2}$	$1-x^2$	$(-1)^n(2n-1)!!$
Jacobi	$P_n^{(\alpha,\beta)}$	$[-1,1]$	$(1-x)^\alpha(x+1)^\beta$	$1-x^2$	$(-1)^n 2^n n!$
Laguerre	L_n	$[0,\infty)$	e^{-x}	x	$n!$
Hermite	H_n	$(-\infty,\infty)$	e^{-x^2}	1	$(-1)^n$

Note that L_n is $L_n^{(0)}$ of **2A.1**.

Exercise. Show $T_n = n!\sqrt{\pi}P_n^{(-1/2,1/2)}/\Gamma(n+1/2)$.

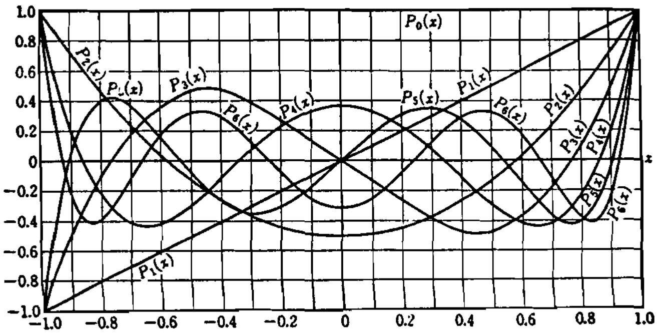
21B.2 Legendre polynomials. The Legendre polynomials have been discussed above (→**21A.5**). The orthonormal basis of $L_2([-1,1])$ (→**20.19**) in terms of the Legendre polynomials is in **21A.5** with the generalized Fourier expansion formula. The decomposition of unity (→**20.15**) reads

$$\delta(x-y) = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(x)P_n(y). \tag{21.35}$$

Rodrigues' formula is in **21A.6**, and the generating function is given in **21A.9**. We can write down the general formula starting from Rodrigues' formula as

$$P_n(x) = \frac{1}{2^n}\sum_{j=0}^{[n/2]} \frac{(-1)^j}{j!}\frac{(2n-2j)!}{(n-j)!(n-2j)!}x^{n-2j}. \tag{21.36}$$

($[\cdot]$ is Gauss' symbol denoting the largest integer not exceeding $\cdot$.)



Discussion.
Let $Q_n(x)$ be the n-th order polynomial with its highest order coefficient normalized to be unity. If its L_2-distance from 0 is the smallest among such polynomials, Q_n is proportional to P_n. That is, minimize

$$\int_{-1}^{1}(x^n + a_{n-1}x^{n-1} + \cdots + a_0)^2 dx \tag{21.37}$$

with respect to the coefficients. The resultant polynomial is proportional to P_n.

21B.3 Sturm-Liouville equation for Legendre polynomials. The differential equation corresponding to (21.16) reads ($\rightarrow$**24C.1**)

$$(1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0, \tag{21.38}$$

or

$$\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}P_n(x)\right] + n(n+1)P_n = 0. \tag{21.39}$$

21B.4 Recursion formulas for Legendre polynomials. The three term recursion relation ($\rightarrow$**21A.10**) reads

$$(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0 \tag{21.40}$$

with $P_0(x) = 1$ and $P_1(x) = x$. This can also be obtained easily from the generating function (21.25): expand

$$(1 - 2x\zeta + \zeta^2)\frac{\partial w}{\partial \zeta} + (-\zeta + x)w = 0. \tag{21.41}$$

Similarly, we obtain

$$(1 - 2x\zeta + \zeta^2)\frac{\partial w}{\partial x} - \zeta w = 0. \tag{21.42}$$

This leads to

$$P_{n+1}' - 2xP_n' + P_{n-1}' - P_n = 0. \tag{21.43}$$

If we eliminate P_{n-1}' from (21.40) and (21.43), we get

$$P_{n+1}' - xP_n' = (n+1)P_n. \tag{21.44}$$

If we eliminate P_{n+1}' from (21.40) and (21.43), we get

$$xP_n' - P_{n-1}' = nP_n. \tag{21.45}$$

Combining above two formulas, we obtain

$$P'_{n+1} - P'_{n-1} = (2n+1)P_n. \tag{21.46}$$

21B.5 Legendre polynomials, some properties.
(1) $P_n(x)$ is an odd (resp., even) function, if n is odd (resp., even): $P_n(x) = (-1)^n P_n(-x)$, $P_n(1) = 1$ and $P_n(-1) = (-1)^n$. $P_{2n}(0) = \binom{-1/2}{n}$ (see Exercise below).
(2) $|P_n(x)| \le 1$.
(3) All the zeros of P_n are simple and in $(-1, 1)$ (→**21A.11**).
(4) If Π_n is an n-th order polynomial satisfying

$$\int_{-1}^{1} \Pi_n(x) x^k dx = 0 \tag{21.47}$$

for all $k \in \{0, 1, \cdots, n-1\}$, then $\Pi_n \propto P_n$ (→**21A.3(2)**).
[Demo of (2)] This can be proved with the aid of Schläfli's integral (21.23). We choose for the intergration path to be

$$t = z + \sqrt{z^2 - 1}e^{i\phi} \tag{21.48}$$

for $\phi \in [-\pi, \pi)$. Note that $dt/(t-z) = id\phi$. Changing the integration variable from t to ϕ in (21.23), we get the following *Laplace's first integral*

$$P_n(x) = \frac{1}{\pi}\int_0^{\pi} [x + \sqrt{x^2-1}\cos\phi]^n d\phi. \tag{21.49}$$

From this we get

$$|P_n(\cos\theta)| \le \frac{1}{\pi}\int_0^{\pi} |\cos\theta + i\sin\theta\cos\phi|^n d\phi \le 1. \tag{21.50}$$

Exercise
$P_{2n}(0)$ can be obtained from Rodrigues' formula (21.11), which reads

$$P_{2n}(0) = (-1)^n \frac{\Gamma(n+1/2)}{\sqrt{\pi}\Gamma(n+1)}. \tag{21.51}$$

21B.6 Hermite polynomials. The orthonormal basis $\{|h_n\rangle\}$ for $L_2((-\infty, \infty), e^{-x^2})$ (→**20.19**) obtained by the Gram-Schmidt method applied to monomials (→**21A.2**) is written in terms of the *Hermite polynomials* $H_n(x)$ as

$$\langle x|h_n\rangle = \sqrt{\frac{1}{2^n n!\sqrt{\pi}}} H_n(x), \tag{21.52}$$

where

$$H_n(x) = \sum_{m=0}^{[(n+1)/2]} (-)^n \frac{n!}{m!(n+1-2m)!}(2x)^{n+1-2m}. \qquad (21.53)$$

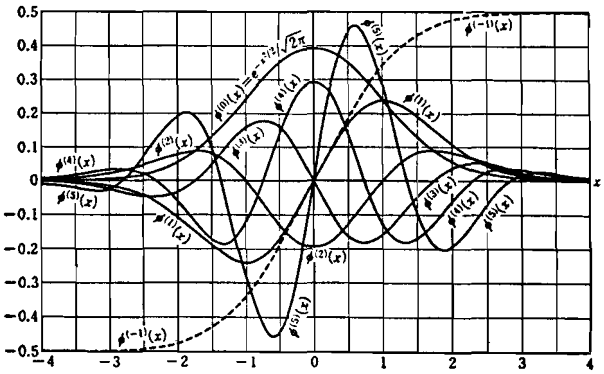
($[\cdot]$ is Gauss' symbol denoting the largest integer not exceeding $\cdot$.) The generalized Rodrigues formula (→**21A.6**) for the Hermite polynomials is

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \qquad (21.54)$$

The generating function (→**21A.8**) is given by

$$W_H(z,\zeta) = e^{2z\zeta-\zeta^2} = \sum_{n=0}^{\infty} \frac{H_n(z)}{n!}\zeta^n. \qquad (21.55)$$

H_n is an even (resp., odd) function, if n is even (resp., odd).



Warning. Many authors use the weight $e^{-x^2/2}$ instead of e^{-x^2}. If we write the Hermite polynomials defined for this weight as $H_n^*(x)$, then the generalized Rodrigues formula (→**21A.6**) reads

$$H_n^*(x) = (-)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2}, \qquad (21.56)$$

and

$$H_n(x) = 2^{n/2} H_n^*(\sqrt{2}x), \quad H_n^*(x) = 2^{-n/2} H_n(x/\sqrt{2}). \qquad (21.57)$$

Discussion.

To demonstrate the completeness of the Hermite polynomials, Weierstrass' theorem **17.3** is not enough, because the latter is about a finite interval. To show the completeness with respect to the L_2-norm we have only to show the completeness of polynomials. This can be demonstrated with the aid of Weierstrass' theorem on increasingly large intervals.

Exercise.
(A) From the generating function show

$$e^{x^2/2}H_n(x) = \frac{1}{i^n\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ixy-y^2/2}H_n(y)dy. \tag{21.58}$$

This can be split into real and imaginary part relations (Lebedev).
(B) From the generating function we obtain the following generalized Fourier expansion

$$e^{ax} = e^{a^2/4}\sum_0^{\infty}\frac{a^n}{2^n n!}H_n(x), \tag{21.59}$$

which is good for all $x \in \boldsymbol{R}$.
(C) Compute the generalized Fourier expansion of e^{-ax^2} in terms of Hermite polynomials. The expansion coefficients can be written as

$$c_{2n} = \frac{1}{2^{2n}(2n)!\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-(a+1)x^2}H_{2n}(x)dx. \tag{21.60}$$

To compute the integral use (21.69) below. The x-integration can be done and we are left with

$$c_{2n} = \frac{(-1)^n a^n}{\sqrt{\pi}(2n)!(1+a)^{n+1/2}}\int_0^{\infty} e^{-s}s^{n-1/2}ds. \tag{21.61}$$

Use the Gamma function ($\to$**9.6**) to obtain the final result (Lebedev)

$$c_{2n} = \frac{(-1)^n a^n}{2^{2n}n!(1+a)^{n+1/2}}. \tag{21.62}$$

21B.7 Sturm-Liouville equation for Hermite polynomials. The formula corresponding to (21.16) reads

$$H_n'' - 2xH_n' + 2nH_n = 0. \tag{21.63}$$

21B.8 Recurrence equations for Hermite polynomials. The three term recurrence relation ($\to$**21A.10**) reads

$$H_{n+1} + 2xH_n + 2nH_{n-1} = 0, \tag{21.64}$$

which can be obtained from

$$\frac{\partial w_H}{\partial \zeta} = -2(z+\zeta)w. \tag{21.65}$$

From

$$\frac{\partial w_H}{\partial z} = 2\zeta w \tag{21.66}$$

we obtain

$$H'_{n+1} = -2(n+1)H_n. \tag{21.67}$$

Exercise.
An integral formula for Hermite polynomials can be obtained with the aid of

$$e^{-x^2} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-t^2} \cos 2xt\, dt. \tag{21.68}$$

[Hint. Note that the integrand is an even function.] Putting this into the generalized Rodrigues' formula (calculate the odd and even n cases separately, and unify the results), we obtain

$$H_n(x) = \frac{2^n(-i)^n e^{x^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-t^2+2itx} t^n dt. \tag{21.69}$$

21B.9 Chebychev polynomials. These polynomials are best introduced as

$$T_n(x) = \cos(n \cos^{-1} x). \tag{21.70}$$

The generalized Rodrigues formula (→**21A.6**) is given by

$$T_n(x) = \frac{(-1)^n}{(2n-1)!!}\sqrt{1-x^2}\frac{d^n}{dx^n}(1-x^2)^{n-1/2}. \tag{21.71}$$

This can be transformed into (21.70) with the aid of the binomial theorem: it is easy to demonstrate that this formula yields

$$\frac{1}{2}[(x + i\sqrt{1-x^2})^n + (x - i\sqrt{1-x^2})^n] \tag{21.72}$$

which reduces to $\cos n\theta$ with $x = \cos\theta$.

The orthonormal basis $\{|t_n\rangle\}$ of $L^2([-1,1], 1/\sqrt{1-x^2})$ (→**20.19**) obtained by the Gram-Schmidt orthonormalization of monomials (→**21A.6**) can be written as

$$\langle x|t_n\rangle = \sqrt{\frac{\pi}{2}} T_n(x). \tag{21.73}$$

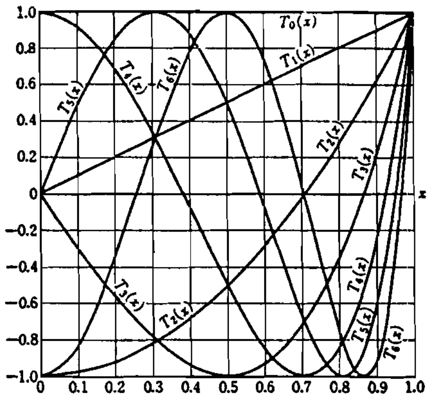
The generating function (→**21A.8**) is

$$\frac{1-z^2}{1-2xz+z^2} = T_0(x) + 2\sum_{n=1}^{\infty} T_n(x) z^n. \tag{21.74}$$

The highest order coefficient of T_n is 2^{n-1} for $n \geq 1$. The three term recursion formula ($\to$**21A.10**) is[315]

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \tag{21.75}$$

for $n = 1, 2, \cdots$ with $T_0 = 1$, $T_1(x) = x$.



Exercise.
(1) Demonstrate that

$$(1 - x^2)T_n''(x) - xT_n'(x) + n^2 T_n(x) = 0. \tag{21.76}$$

(2) Demonstrate the generating function for Chebychev polynomials (21.74) as elegantly as possible. [Hint. Use ( ).]
21.70

21B.10 Remarkable properties of Chebychev polynomials.

(1) Theorem. Let $p_n(x)$ be a polynomial of order $n (\geq 1)$ whose coefficient of x^n is unity. Then,

$$\max_{x \in [-1,1]} |p_n(x)| \geq 2^{1-n}, \tag{21.77}$$

and the equality holds if and only if $p_n(x) = T_n(x)/2^{n-1}$.□
(2) The best (w.r.t. the sup norm) n-th order polynomial approximant of x^{n+1} on $[-1, 1]$ is given by $T_{n+1}(x)/2^n - x^{n+1}$. This property makes the Chebychev polynomial very important in approximation theory of functions.
(3) $x_{k+1} = T_n(x_k)$ defines a sequence $x_0, x_1, x_2, \cdots$ from the initial condition x_0. This is a typical chaotic sequence. Among any continuous functions with n laps, $T_n(x)$ gives the most chaotic sequences on the average.

[315] This is nothing but $\cos(n+1)x + \cos(n-1)x = 2\cos x \cos nx$.

Discussion.

(A) (1) above implies that if the n-th order polynomial Q_n defined on $[-1, 1]$ with its highest order coefficient normalized to be unity and if its maximum deviation from zero is the smallest among such polynomials, then Q_n is proportional to the order n Chebychev polynomial.

(B) Take $T_2(x)$. Demonstrate that there are two intervals I and J in $[-1, 1]$ which share at most one point such that $T_2(I) \cap T_2(J) \supset I \cup J$. In general, if the reader can find two positive integers and two intervals I and J sharing at most one point such that $f^n(I) \cap f^m(J) \supset I \cup J$, then f exhibits chaos on the inteval containing both I and J. That is, there is an invariant set Ω of f^N for some positive integer N such that f^N restricted to Ω is isomorphic to the coin-tossing process.).