Χρησιμα Key 6 & Key 7

Table 7.1 Roots of the Wilkinson polynomial (7.2.12) with $\varepsilon = 10^{-9}$

The first column lists the unperturbed ($\varepsilon = 0$) roots 1, 2, ..., 20; the second column gives the results of first-order perturbation theory (see Prob. 7.22); the third column gives the exact roots. The unperturbed roots at 13 and 14, 15 and 16, and 17 and 18 are perturbed into complex-conjugate pairs. Observe that while first-order perturbation theory is moderately accurate for the real perturbed roots near 1, 2, ..., 12, 19, 20, it cannot predict the locations of the complex roots (but see Prob. 7.23)

Unperturbed root	First-order perturbation theory	Exact root
1	1.000 000 000 0	1.000 000 000 0
2	2.000 000 000 0	2.000 000 000 0
3	3.000 000 000 0	3.000 000 000 0
4	4.000 000 000 0	4.000 000 000 0
5	5.000 000 000 0	5.000 000 000 0
6	5.999 999 941 8	5.999 999 941 8
7	7.000 002 542 4	7.000 002 542 4
8	7.999 994 030 4	7.999 994 031 5
9	9.000 839 327 5	9.000 841 033 5
10	9.992 405 941 6	9.992 518 124 0
11	11.046 444 571	11.050 622 592
12	11.801 496 835	11.832 935 987
13	13.605 558 629	$13.349\,018\,036 \pm 0.532\,765\,750\,0i$
14	12.667 031 557	
15	17.119 065 220	$15.457\,790\,724 \pm 0.899\,341\,526\,2i$
16	13.592 486 027	
17	18.904 402 150	$17.662\,434\,477 \pm 0.704\,285\,236\,9i$
18	17.004 413 300	
19	19.309 013 459	19.233 703 334
20	19.956 900 195	19.950 949 654

This example shows that the roots of high-degree polynomials may be extraordinarily sensitive to changes in the coefficients of the polynomial, even though the perturbation problem so obtained is regular. It should serve as ample warning to a "number cruncher" not to trust computer output without sufficient understanding of the nature of the problem being solved.

(I) 7.3 PERTURBATION METHODS FOR LINEAR EIGENVALUE PROBLEMS

In this section we show how perturbation theory can be used to approximate the eigenvalues and eigenfunctions of the Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + V(x) + W(x) - E\right] y(x) = 0, \tag{7.3.1}$$

subject to the boundary condition

$$\lim_{|x|\to\infty} y(x) = 0. \tag{7.3.2}$$

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« Asymptotic Methods and Perturbation Theory »

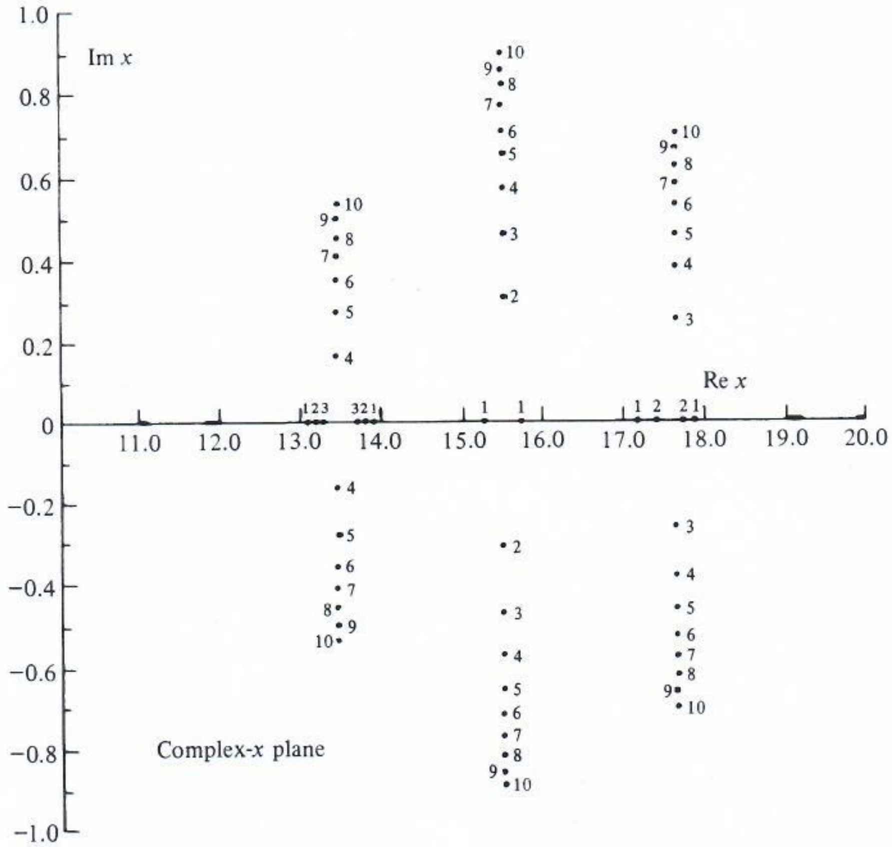

Figure 7.5 Roots of the Wilkinson polynomial $(x-1)(x-2)(x-3)\cdots(x-20)+\varepsilon x^{19}$ in (7.2.12) for 11 values of ε. When $\varepsilon = 0$ the roots shown are 10, 11, . . . , 20. As ε is allowed to increase very slowly, the roots move toward each other in pairs along the real-x axis and then veer off in opposite directions into the complex-x plane. We have plotted the roots for $\varepsilon = 0, 10^{-10}, 2\times 10^{-10}, 3\times 10^{-10}, \ldots, 10^{-9}$. Some of the roots are numbered to indicate the value of ε to which they correspond; that is, 6 means $\varepsilon = 6\times 10^{-10}$, 3 means $\varepsilon = 3\times 10^{-10}$, and so on. The roots starting at 11, 12, 19, and 20 move too slowly to be seen as individual dots. We conclude from this plot that very slight changes in the coefficients of a polynomial can cause drastic changes in the values of some of the roots; one must be cautious when performing numerical calculations.

In (7.3.1) E is called the energy eigenvalue and $V + W$ is called the potential. We assume that $V(x)$ and $W(x)$ are continuous functions and that both $V(x)$ and $V(x) + W(x)$ approach ∞ as $|x| \to \infty$.

We suppose that the function $V(x) + W(x)$ is so complicated that (7.3.1) is not soluble in closed form. One can still prove from the above assumptions that nontrivial solutions $[y(x) \not\equiv 0]$ satisfying (7.3.1) and (7.3.2) exist for special discrete values of E, the allowed eigenvalues of the equation (see Sec. 1.8). On the other hand, we assume that removing the term $W(x)$ from (7.3.1) makes the equation an

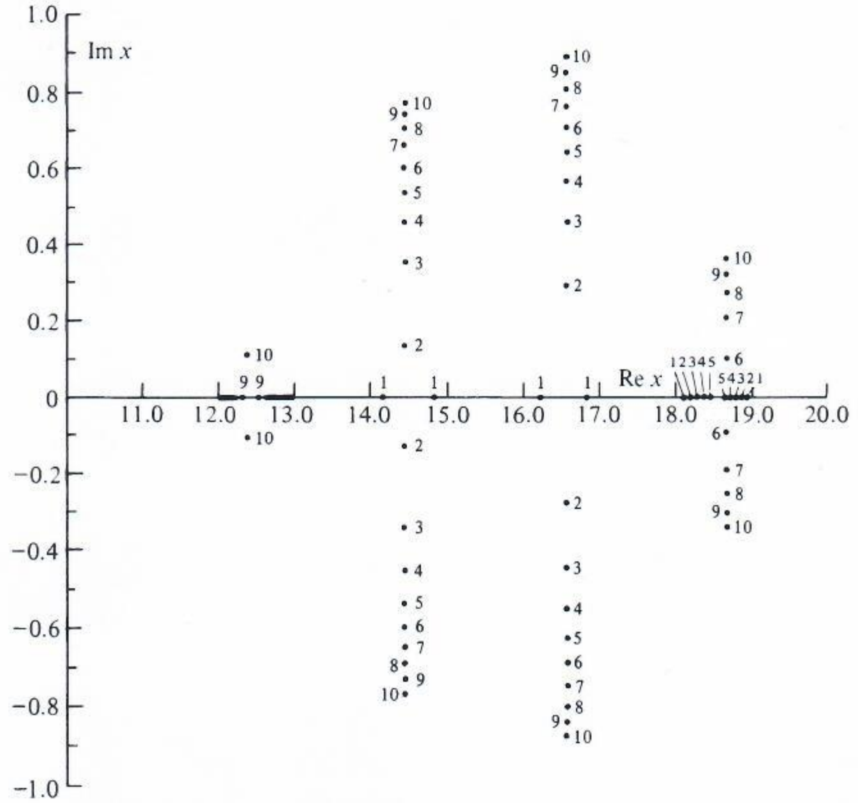

Figure 7.6 Same as in Fig. 7.5 except that the values of ε are 0, -10^{-10}, -2×10^{-10}, $-3 \times 10^{-10}, \ldots, -10^{-9}$. The roots pair up and veer off into the complex-x plane, but the pairs are not the same as in Fig. 7.5.

exactly soluble eigenvalue problem. This suggests using perturbation theory to solve the family of eigenvalue problems in which $W(x)$ is replaced by $\varepsilon W(x)$:

$$\left[-\frac{d^2}{dx^2} + V(x) + \varepsilon W(x) - E\right] y(x) = 0. \tag{7.3.3}$$

Our assumptions on the nature of $V(x)$ and $W(x)$ leave no choice about where to introduce the parameter ε if the unperturbed problem is to be exactly soluble.

Example 1 *An exactly soluble eigenvalue problem.* Several exactly soluble eigenvalue problems are given in Sec. 1.8. One such example, which is used extensively in this section, is obtained if we take $V(x) = x^2/4$. The unperturbed problem is the Schrödinger equation for the quantum-mechanical harmonic oscillator, which is just the parabolic cylinder equation

$$-y'' + \frac{x^2}{4} y - Ey = 0. \tag{7.3.4}$$

We have already shown that solutions to this equation behave like $e^{\pm x^2/4}$ as $|x| \to \infty$.

There is a discrete set of values of E for which a solution that behaves like $e^{-x^2/4}$ as $x \to \infty$ also behaves like $e^{-x^2/4}$ as $x \to -\infty$ (see Example 4 of Sec. 3.5 and Example 9 of Sec. 3.8). These values of E are

$$E = n + \tfrac{1}{2}, \qquad n = 0, 1, 2, \ldots, \tag{7.3.5}$$

and the associated eigenfunctions are parabolic cylinder functions

$$y_n(x) = D_n(x) = e^{-x^2/4}\,\mathrm{He}_n(x), \tag{7.3.6}$$

where $\mathrm{He}_n(x)$ is the Hermite polynomial of degree n: $\mathrm{He}_0(x) = 1$, $\mathrm{He}_1(x) = x$, $\mathrm{He}_2(x) = x^2 - 1, \ldots$.

In general, once an eigenvalue E_0 and an eigenfunction $y_0(x)$ of the unperturbed problem

$$\left[-\frac{d^2}{dx^2} + V(x) - E_0\right] y_0(x) = 0 \tag{7.3.7}$$

have been found, we may seek a perturbative solution to (7.3.3) of the form

$$E = \sum_{n=0}^{\infty} E_n \varepsilon^n, \tag{7.3.8}$$

$$y(x) = \sum_{n=0}^{\infty} y_n(x)\varepsilon^n. \tag{7.3.9}$$

Substituting (7.3.8) and (7.3.9) into (7.3.3) and comparing powers of ε gives the following sequence of equations:

$$\left[-\frac{d^2}{dx^2} + V(x) - E_0\right] y_n(x) = -Wy_{n-1}(x) + \sum_{j=1}^{n} E_j y_{n-j}(x), \qquad n = 1, 2, 3, \ldots, \tag{7.3.10}$$

whose solutions must satisfy the boundary conditions

$$\lim_{|x| \to \infty} y_n(x) = 0, \qquad n = 1, 2, 3, \ldots. \tag{7.3.11}$$

Equation (7.3.10) is linear and inhomogeneous. The associated homogeneous equation is just the unperturbed problem and thus is soluble by assumption. However, technically speaking, only *one* of the two linearly independent solutions of the unperturbed problem (the one that satisfies the boundary conditions) is assumed known. Therefore, we proceed by the method of reduction of order (see Sec. 1.4); to wit, we substitute

$$y_n(x) = y_0(x)F_n(x), \tag{7.3.12}$$

where $F_0(x) = 1$, into (7.3.10). Simplifying the result using (7.3.7) and multiplying by the integrating factor $y_0(x)$ gives

$$\frac{d}{dx}[y_0^2(x)F_n'(x)] = y_0^2(x)\left[W(x)F_{n-1}(x) - \sum_{j=1}^{n} E_j F_{n-j}(x)\right]. \tag{7.3.13}$$

If we integrate this equation from $-\infty$ to ∞ and use $y_0^2(x)F_n'(x) = y_0(x)y_n'(x) - y_0'(x)y_n(x) \to 0$ as $|x| \to \infty$, we obtain the formula for the coefficient E_n:

$$E_n = \frac{\displaystyle\int_{-\infty}^{\infty} y_0(x)\left[W(x)y_{n-1}(x) - \sum_{j=1}^{n-1} E_j y_{n-j}(x)\right] dx}{\displaystyle\int_{-\infty}^{\infty} y_0^2(x)\, dx}, \qquad n = 1, 2, 3, \ldots, \tag{7.3.14}$$

from which we have eliminated all reference to $F_n(x)$. [The sum on the right side of (7.3.14) is defined to be 0 when $n = 1$.]

Integrating (7.3.13) twice gives the formula for $y_n(x)$:

$$y_n(x) = y_0(x) \int_a^x \frac{dt}{y_0^2(t)} \int_{-\infty}^{t} ds\, y_0(s)\left[W(s)y_{n-1}(s) - \sum_{j=1}^{n} E_j y_{n-j}(s)\right], \qquad n = 1, 2, 3, \ldots. \tag{7.3.15}$$

Observe that in (7.3.15) a is an arbitrary number at which we choose to impose $y_n(a) = 0$. This means we have fixed the overall normalization of $y(x)$ so that $y(a) = y_0(a)$ [assuming that $y_0(a) \neq 0$]. If $y_0(t)$ vanishes between a and x, the integral in (7.3.15) seems formally divergent; however, $y_n(x)$ satisfies a differential equation (7.3.10) which has no finite singular points. Thus, it is possible to define $y_n(x)$ everywhere as a finite expression (see Prob. 7.24).

Equations (7.3.14) and (7.3.15) together constitute an iterative procedure for calculating the coefficients in the perturbation series for E and $y(x)$. Once the coefficients $E_0, E_1, \ldots, E_{n-1}, y_0, y_1, \ldots, y_{n-1}$ are known, (7.3.14) gives E_n, and once E_n has been calculated (7.3.15) gives y_n. The remaining question is whether or not these perturbation series are convergent.

Example 2 *A regular perturbative eigenvalue problem.* Let $V(x) = x^2/4$ and $W(x) = x$. It may be shown (Prob. 7.25) that the perturbation series for $y(x)$ is convergent for all ε and that the series for E has vanishing terms of order ε^n for $n \geq 3$. This is a regular perturbation problem.

Example 3 *A singular perturbative eigenvalue problem.* It may be shown (Prob. 7.26) that if $V(x) = x^2/4$ and $W(x) = x^4/4$, then the perturbation series for the smallest eigenvalue for positive ε is

$$E(\varepsilon) \sim \tfrac{1}{2} + \tfrac{3}{4}\varepsilon - \tfrac{21}{8}\varepsilon^2 + \tfrac{333}{16}\varepsilon^3 + \cdots, \qquad \varepsilon \to 0+. \tag{7.3.16}$$

The terms in this series appear to be getting larger and suggest that this series may be divergent for all $\varepsilon \neq 0$. Indeed, (7.3.16) diverges for all ε because the nth term satisfies $E_n \sim -(-3)^n\Gamma(n + \frac{1}{2})\sqrt{6}/\pi^{3/2}$ $(n \to \infty)$. (This is a nontrivial result that we do not explain here.)

The divergence of the perturbation series in Example 3 indicates that the perturbation problem is singular. A simple way to observe the singular behavior is to compare $e^{-x^2/4}$, the controlling factor of the large-x behavior of the unperturbed ($\varepsilon = 0$) solution, with $e^{-x^3\sqrt{\varepsilon}/6}$, the controlling factor of the large-x behavior for $\varepsilon \neq 0$. There is an abrupt change in the nature of the solution when we pass to the limit ($\varepsilon \to 0+$). This phenomenon occurs because the perturbing term $\varepsilon x^4/4$ is not small compared with $x^2/4$ when x is large.

If the functions $V(x)$ and $W(x)$ in Example 3 were interchanged, then the resulting eigenvalue problem would be a regular perturbation problem because εx^2 is a small perturbation of x^4 for all $|x| < \infty$. However, the unperturbed problem, $(-d^2/dx^2 + x^4/4 - E_0)y_0(x) = 0$, is not soluble in closed form. Thus, it would not be possible to use (7.3.14) and (7.3.15) to compute the coefficients in the perturbation series analytically.

Also note that if the boundary conditions in Example 3 were given at $x = \pm A$, $A < \infty$, then the perturbation theory would be regular. This is because here εx^4 is a small perturbation of x^2. However, it is much more difficult to solve the unperturbed problem on a finite interval.

Thus, one is forced to accept a solution to Example 3 in the form of a divergent series. Fortunately, this series is one of many that may be summed by Padé theory to give a finite and unique result (see Sec. 8.3).

Example 4 *Another regular perturbation problem.* When $V = x^2/4$ and $W = |x|$ the perturbation problem is regular. But unlike the problem in Example 2, this perturbation series is not convergent for all ε; the series in (7.3.8) and (7.3.9) have finite radii of convergence. The significance of the finite radius of convergence is discussed in Sec. 7.5.

(D) 7.4 ASYMPTOTIC MATCHING

The purpose of this section is to introduce the notion of matched asymptotic expansions. Asymptotic matching is an important perturbative method which is used often in both boundary-layer theory (Chap. 9) and WKB theory (Chap. 10) to determine analytically the approximate global properties of the solution to a differential equation. Asymptotic matching is usually used to determine a uniform approximation to the solution of a differential equation and to find other global properties of differential equations such as eigenvalues. Asymptotic matching may also be used to develop approximations to integrals.

The principle of asymptotic matching is simple. The interval on which a boundary-value problem is posed is broken into a sequence of two or more *overlapping* subintervals. Then, on each subinterval perturbation theory is used to obtain an asymptotic approximation to the solution of the differential equation valid on that interval. Finally, the matching is done by requiring that the asymptotic approximations have the same functional form on the overlap of every pair of intervals. This gives a sequence of asymptotic approximations to the solution of the differential equation; by construction, each approximation satisfies all the boundary conditions given at various points on the interval. Thus, the end result is an approximate solution to a boundary-value problem valid over the entire interval.

Asymptotic matching bears a slight resemblance to an elementary technique for solving boundary-value problems called *patching*. Patching is helpful when the differential equation can be solved in closed form. Here is a simple example:

Example 1 *Patching.* The method of patching may be used to solve the boundary-value problem $y'' - y = e^{-|x|}$ $[y(\pm\infty) = 0]$. There are two regions to consider. When $x \le 0$, the most general solution which satisfies the boundary condition $y(-\infty) = 0$ is

$$y(x) = ae^x + \tfrac{1}{2}xe^x, \tag{7.4.1}$$