Introduction to Optical Waveguide Analysis: Solving Maxwell's Equations and the Schrödinger Equation. Kenji Kawano, Tsutomu Kitoh
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CHAPTER 7

SCHRÖDINGER EQUATION

In this chapter, we will investigate ways to solve the Schrödinger equation, which must be solved when quantum wells for semiconductor optical waveguide devices are designed [1, 2]. The time-dependent Schrödinger equation resembles the Fresnel wave equation, and the time-independent Schrödinger equation resembles the wave equation for the cross-sectional analysis. Thus, the analysis techniques given earlier for optical waveguides can be applied to the analysis of these Schrödinger equations. Here, the analysis of the time-dependent Schrödinger equation will be based on the 2D FD-BPM and the analysis of the time-independent Schrödinger equation will be based on the 1D FDM and the 1D FEM.

7.1 TIME-DEPENDENT STATE

Let us solve the time-dependent Schrödinger equation by using the 2D FD-BPM. The only major difference between the time-dependent Schrödinger equation and the BPM wave equation based on the Fresnel approximation is that the derivative in the Schrödinger equation is with respect to time, whereas the derivative in the BPM wave equation is with respect to position.

Under the effective mass approximation, the time-dependent Schrödinger equation is expressed as

$$j\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left(\frac{1}{m(x)}\frac{\partial \psi(x,t)}{\partial x}\right) + U(x)\psi(x,t), \tag{7.1}$$

where $U(x)$, $m(x)$, and $\hbar$ are respectively an arbitrary potential shown in Fig. 7.1, an effective mass, and the Plank constant [3].

First, the time t and the space x are discretized. The nonequidistant discretization shown in Fig. 5.5 is assumed, and the wave function $\psi(x, t)$, the potential $U(x)$, and the effective mass $m(x)$ are expressed as

$$\psi(x,t) = \psi(x_p, t_n) = \psi_p^n, \tag{7.2}$$

$$U(x) = U(x_p) = U(p), \tag{7.3}$$

$$m(x) = m(x_p) = m(p). \tag{7.4}$$

The 2D Fresnel wave equation for the TM mode of an optical waveguide that was derived in Chapter 5 [Eq. (5.118)] is

$$2j\beta \frac{\partial \phi(x,z)}{\partial z} = \varepsilon_r(x)\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon_r(x)}\frac{\partial \phi(x,z)}{\partial x}\right) + k_0^2[\varepsilon_r(x) - n_{\text{eff}}^2]\phi(x,z). \tag{7.5}$$

Comparing this with the time-dependent Schrödinger equation (7.1), we find the following correspondences:

$$z \leftrightarrow t, \tag{7.6}$$

$$\varepsilon_r(x)\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon_r(x)}\frac{\partial}{\partial x}\right) \leftrightarrow -\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left(\frac{1}{m(x)}\frac{\partial}{\partial x}\right), \tag{7.7}$$

$$2j\beta \leftrightarrow j\hbar, \tag{7.8}$$

$$k_0^2[\varepsilon_r(x) - n_{\text{eff}}^2] \leftrightarrow U(x). \tag{7.9}$$

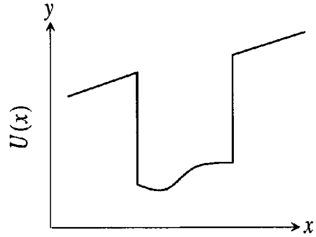

FIGURE 7.1. Potential distribution for a semiconductor quantum well.

Thus, from Eq. (5.126) and Eqs. (5.142)–(5.144), we can get the finite-difference expression for the right-hand side of correspondence (7.7):

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left(\frac{1}{m(x)}\frac{\partial\phi}{\partial x}\right) = \alpha_w\psi_{p-1} + \alpha_x\psi_p + \alpha_e\psi_{p+1}, \tag{7.10}$$

where

$$\alpha_w = -\frac{\hbar^2}{2}\frac{2}{w(e+w)}\frac{2}{m(p)+m(p-1)}, \tag{7.11}$$

$$\alpha_e = -\frac{\hbar^2}{2}\frac{2}{e(e+w)}\frac{2}{m(p)+m(p+1)}, \tag{7.12}$$

$$\begin{aligned}\alpha_x &= \frac{\hbar^2}{2}\left(\frac{2}{w(e+w)}\frac{2}{m(p)+m(p-1)}\right.\\ &\qquad\left.+\frac{2}{e(e+w)}\frac{2}{m(p)+m(p+1)}\right)\\ &= -\alpha_e - \alpha_w.\end{aligned} \tag{7.13}$$

Considering the relations shown in correspondences (7.6)–(7.9) and in Eq. (5.135), we get the following finite-difference expression for the time-dependent Schrödinger equation:

$$\begin{aligned}&-\alpha_w\psi_{p-1}^{n+1} + \left(-\alpha_x + \frac{2j\hbar}{\Delta t} - U(p)\right)\psi_p^{n+1} - \alpha_e\psi_{p+1}^{n+1}\\ &= \alpha_w\psi_{p-1}^{l} + \left(\alpha_x + \frac{2j\hbar}{\Delta t} + U(p)\right)\psi_p^{l} + \alpha_e\psi_{p+1}^{l}.\end{aligned} \tag{7.14}$$

It is easily understood that this equation can be solved in the same way that the 2D FD-BPM is solved and that the transparent boundary condition can also be used with this equation.

7.2 FINITE-DIFFERENCE ANALYSIS OF TIME-INDEPENDENT STATE

The wave function $\psi(x, t)$ that satisfies the time-dependent Schrödinger equation (7.1) is divided into the space-dependent term and the time-dependent term as follows:

$$\psi(x, t) = \phi(x)\exp(-j\omega t) = \phi(x)\exp\left(-jE\frac{t}{\hbar}\right), \tag{7.15}$$

where E is the eigenenergy to be calculated and corresponds to the effective index in the optical waveguide problems.

Substituting Eq. (7.15) into Eq. (7.1) and dividing the resultant equation by $\exp(-jEt/\hbar)$, we get

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d\phi(x)}{dx}\right) + [U(x) - E]\phi(x) = 0. \tag{7.16}$$

This is the time-independent Schrödinger equation. Discretizing it by using Eqs. (7.10)–(7.13), we get the following finite-difference expression:

$$\alpha_w\phi_{p-1} + \alpha_e\phi_{p+1} + \alpha_x\phi_p + [U(p) - E]\phi_p = 0$$

and therefore

$$\alpha_w\phi_{p-1} + [\alpha_x + U(p)]\phi_p + \alpha_e\phi_{p+1} - E\phi_p = 0. \tag{7.17}$$

The remaining task is to construct a matrix equation for Eq. (7.17).

7.3 FINITE-ELEMENT ANALYSIS OF TIME-INDEPENDENT STATE

7.3.1 Eigenvalue Equation

To solve the time-independent Schrödinger equation, we first derive the eigenvalue equation based on the FEM [4, 5]. The following normalizations are introduced:

$$\bar{x} = \frac{x}{W} \quad \text{(coordinate)}, \tag{7.18}$$

$$\bar{U}(\bar{x}) = \frac{U(x)}{E_1^\infty} \quad \text{(potential)}, \tag{7.19}$$

$$\bar{E} = \frac{E}{E_1^\infty} \quad \text{(eigenenergy)}, \tag{7.20}$$

$$\bar{m} = \frac{m(x)}{m_0} \quad \text{(effective mass)}, \tag{7.21}$$

where $E_1^\infty = \hbar^2\pi^2/(2m_0W^2)$, m_0, and W are respectively the electron energy of the ground state in an infinitely deep well, the static mass of an electron, and the width of a quantum well.

When we substitute these normalized parameters into Eq. (7.16), we get the normalized Schrödinger equation

$$-\frac{d}{d\bar{x}}\left(\frac{1}{m(\bar{x})}\frac{d\phi(\bar{x})}{d\bar{x}}\right) + \pi^2[\bar{U}(\bar{x}) - \bar{E}]\phi(\bar{x}) = 0. \tag{7.22}$$

Next, we use the Galerkin method to solve this equation. For simplicity, the overbar, denoting normalized quantities in Eqs. (7.18) to (7.22), is omitted. Figure 7.2 shows nodes used in the 1D FEM. Using shape functions, we expand the wave function $\phi(x)$ for an element e:

$$\phi_e = \sum_{i=1}^{M_e} N_{ei}\phi_{ei} = [N_e]^T\{\phi_e\}. \tag{7.23}$$

Substituting Eq. (7.23) into Eq. (7.22), we get

$$-\frac{d}{dx}\left(\frac{1}{m_e}\frac{d}{dx}\right)[N_e]^T\{\phi_e\} + \pi^2[U(x) - E][N_e]^T\{\phi_e\} = 0.$$

Multiplying the left-hand side of this equation by the shape function and integrating the resultant equation in element e, we get

$$-\int_e [N_e]\frac{d}{dx}\left(\frac{1}{m_e}\frac{d}{dx}\right)[N_e]^T\, dx\{\phi_e\}$$
$$+ \pi^2\int_e [N_e][U(x) - E][N_e]^T\, dx\{\phi_e\} = \{0\}. \tag{7.24}$$

Applying the partial integration to the first term of Eq. (7.24) and denoting the node numbers of the left- and right-hand nodes in element e as i and $i+1$, we rewrite Eq. (7.24) as

$$-\left[[N_e]\frac{1}{m_e}\frac{d[N_e]^T}{dx}\{\phi_e\}\right]_i^{i+1} + \int_e \frac{d[N_e]}{dx}\frac{1}{m_e}\frac{d[N_e]^T}{dx}\, dx\{\phi_e\}$$
$$+ \pi^2\int_e [N_e](U(x) - E)[N_e]^T\, dx\{\phi_e\} = \{0\}.$$

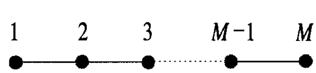

FIGURE 7.2. Nodes in the 1D finite-element method.

Furthermore, assuming that both the effective mass m and the potential $U(x)$ ($=U_e$) are constant in the element, we can reduce this equation to

$$-\left[[N_e]\frac{1}{m_e}\frac{d[N_e]^T}{dx}\{\phi_e\}\right]_i^{i+1}+\int_e\frac{1}{m_e}\frac{d[N_e]}{dx}\frac{d[N_e]^T}{dx}\,dx\{\phi_e\}$$
$$+\pi^2(U_e-E)\int_e[N_e][N_e]^T\,dx\{\phi_e\}=\{0\}. \tag{7.25}$$

Next, we sum Eq. (7.25) for all elements. The first term of Eq. (7.25) becomes

$$\begin{aligned}
&\sum_e\left[[N_e]\frac{1}{m}\frac{d[N_e]^T}{dx}\{\phi_e\}\right]_i^{i+1}\\
&=\left(\phi_2\frac{1}{m_2}\frac{d\phi_2}{dx}-\phi_1\frac{1}{m_1}\frac{d\phi_1}{dx}\right)+\left(\phi_3\frac{1}{m_3}\frac{d\phi_3}{dx}-\phi_2\frac{1}{m_2}\frac{d\phi_2}{dx}\right)+\cdots\\
&\quad+\left(\phi_{M-1}\frac{1}{m_{M-1}}\frac{d\phi_{M-1}}{dx}-\phi_{M-2}\frac{1}{m_{M-2}}\frac{d\phi_{M-2}}{dx}\right)\\
&\quad+\left(\phi_M\frac{1}{m_M}\frac{d\phi_M}{dx}-\phi_{M-1}\frac{1}{m_{M-1}}\frac{d\phi_{M-1}}{dx}\right)\\
&=-\phi_1\frac{1}{m_1}\frac{d\phi_1}{dx}+\phi_M\frac{1}{m_M}\frac{d\phi_M}{dx},
\end{aligned}$$

where M is the total number of nodes. It should be noted that the following continuity conditions for the wave function and its derivative are assumed at adjacent elements e and $e+1$:

$$\phi|_e=\phi|_{e+1},\qquad \left.\frac{1}{m}\frac{\partial\phi}{\partial x}\right|_e=\left.\frac{1}{m}\frac{\partial\phi}{\partial x}\right|_{e+1}. \tag{7.26}$$

Thus, after summing Eq. (7.25) for all elements, we get

$$\left(\phi_1\frac{1}{m_1}\frac{d\phi_1}{dx}-\phi_M\frac{1}{m_M}\frac{d\phi_M}{dx}\right)+\sum_e\frac{1}{m_e}\int_e\frac{d[N_e]}{dx}\frac{d[N_e]^T}{dx}\,dx\{\phi_e\}$$
$$+\pi^2\sum_e U_e\int_e[N_e][N_e]^T\,dx\{\phi_e\}-\pi^2E\sum_e\int_e[N_e][N_e]^T\,dx\{\phi_e\}=\{0\}. \tag{7.27}$$

This equation can be reduced to

$$\left(\phi_1 \frac{1}{m_1} \frac{d\phi_1}{dx} - \phi_M \frac{1}{m_M} \frac{d\phi_M}{dx}\right) + [P]\{\phi\} + \pi^2[Q]\{\phi\} - \pi^2 E[R]\{\phi\} = \{0\}, \tag{7.28}$$

where

$$[P] = \sum_e \frac{1}{m_e} \int_e \frac{d[N_e]}{dx} \frac{d[N_e]^T}{dx}\, dx, \tag{7.29}$$

$$[Q] = \sum_e U_e \int_e [N_e][N_e]^T\, dx, \tag{7.30}$$

$$[R] = \sum_e \int_e [N_e][N_e]^T\, dx, \tag{7.31}$$

$$\{\phi\} = \sum_e \{\phi_e\}. \tag{7.32}$$

Assuming the Dirichlet condition or the Neumann condition—that is, assuming

$$\phi = 0 \tag{7.33}$$

or

$$\frac{d\phi}{dx} = 0 \tag{7.34}$$

at the leftmost node 1 and the rightmost node M—we can obtain from Eq. (7.28) the simple eigenvalue equation

$$([P] + \pi^2[Q])\{\phi\} - E(\pi^2[R])\{\phi\} = \{0\}. \tag{7.35}$$

To solve this equation, we have to transform Eqs. (7.28) and (7.35) into eigenvalue matrix equations. To this end, in the following, the first- and second-order shape functions will be obtained and the explicit expressions for the matrixes will be shown.

7.3.2 Matrix Elements

A. First-Order Line Element The matrixes for the eigenvalue equation will be calculated by using the first-order line element. Figure 7.3 shows the first-order line element. The node numbers i and j and the coordinates x_i and x_j are assumed to correspond to the local coordinates 1 and 2. An arbitrary coordinate x in element e is defined using the parameter ξ, which takes a value between 0 and 1:

$$x = (1 - \xi)x_i + \xi x_j = x_i + (x_j - x_i)\xi = x_i + L_e\xi, \tag{7.36}$$

where L_e is the length of the element $(x_j - x_i)$. Since the first-order line element has two nodes, the wave function $\phi_e(x)$ in element e is expanded as

$$\phi_e(x) = \sum_{i=1}^{2} N_i(\xi)\phi_i = [N]^T\{\phi_e\} \tag{7.37}$$

by using the shape function $[N]^T$. The shape functions N_1 and N_2 for the line elements are expressed by the linear functions

$$N_1(\xi) = a_1\xi + b_1, \qquad N_2(\xi) = a_2\xi + b_2, \tag{7.38}$$

and the conditions that must be met by the shape functions are

$$\xi = 0: \qquad N_1(0) = 1, \qquad N_2(0) = 0, \tag{7.39}$$

$$\xi = 1: \qquad N_1(1) = 0, \qquad N_2(1) = 1. \tag{7.40}$$

Thus, the following shape functions can be obtained for the first-order line element:

$$N_1(\xi) = 1 - \xi, \tag{7.41}$$

$$N_2(\xi) = \xi. \tag{7.42}$$

Next, we calculate the matrix elements shown in Eqs. (7.29)–(7.32).

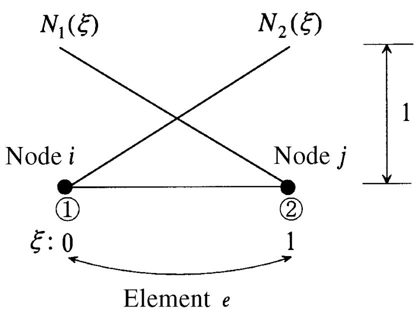

FIGURE 7.3. First-order line element.

1. $\int_e (d[N_e]/dx)(d[N_e]^T/dx)\,dx$ From Eq. (7.36), we get

$$\frac{d\xi}{dx} = \frac{1}{L_e}$$

and therefore,

$$dx = L_e\,d\xi. \tag{7.43}$$

Since the relations

$$\frac{dN_1}{d\xi} = -1, \tag{7.44}$$

$$\frac{dN_2}{d\xi} = 1, \tag{7.45}$$

hold, we get

$$\frac{d[N_e]}{dx} = \frac{d\xi}{dx}\,\frac{d[N_e]}{d\xi} = \frac{1}{L_e}\begin{bmatrix} -1 \\ 1 \end{bmatrix}. \tag{7.46}$$

Thus, we get

$$\begin{aligned}\int_e \frac{d[N_e]}{dx}\,\frac{d[N_e]^T}{dx}\,dx &= \frac{1}{L_e^2}\int_0^1 \begin{bmatrix} -1 \\ 1 \end{bmatrix}[-1 \quad 1]L_e\,d\xi \\ &= \frac{1}{L_e}\int_0^1 \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} d\xi \\ &= \frac{1}{L_e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \end{aligned} \tag{7.47}$$

2. $\int_e [N_e][N_e]^T\,dx$ Through a similar procedure, we get

$$\begin{aligned}\int_e [N_e][N_e]^T\,dx &= \int_0^1 \begin{bmatrix} (1-\xi) \\ \xi \end{bmatrix}[(1-\xi) \quad \xi]L_e\,d\xi \\ &= L_e\int_0^1 \begin{bmatrix} (1-\xi)^2 & \xi(1-\xi) \\ \xi(1-\xi) & \xi^2 \end{bmatrix} d\xi = \frac{L_e}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}. \end{aligned} \tag{7.48}$$

Since Eqs. (7.47) and (7.48) can be used to construct the matrixes [P], [Q], and [R], the eigenenergy can be calculated from the eigenvalue matrix equation (7.35).

B. Second-Order Line Element Next, we discuss the second-order line element, which is more accurate than the first-order line element. Figure 7.4 shows the second-order line element. The node numbers i, j, and k and the coordinates x_i, x_j, and x_k are assumed to correspond to the local coordinates 1, 2, and 3. An arbitrary coordinate x in element e is defined using the parameter ξ, which takes a value between -1 and 1:

$$x = x_j + \tfrac{1}{2}(x_k - x_i)\xi. \tag{7.49}$$

Since the second-order line element has three nodes, the wave function $\phi_e(x)$ in element e is expanded as

$$\phi_e(x) = \sum_{i=1}^{3} N_i(\xi)\phi_i = [N_e]^T\{\phi_e\} \tag{7.50}$$

by using the shape function $[N]^T$. The shape functions N_1, N_2, and N_3 for the line elements are expressed by the quadratic polynomials

$$\begin{aligned} N_1(\xi) &= a_1\xi^2 + b_1\xi + c_1, \\ N_2(\xi) &= a_2\xi^2 + b_2\xi + c_2, \\ N_3(\xi) &= a_3\xi^2 + b_3\xi + c_3, \end{aligned} \tag{7.51}$$

and the conditions that must be met by the shape functions are

$$\xi = 0: \qquad N_1(0) = 0, \qquad N_2(0) = 1, \qquad N_3 = 0, \tag{7.52}$$

$$\xi = 1: \qquad N_1(1) = 0, \qquad N_2(1) = 0, \qquad N_3(1) = 1, \tag{7.53}$$

$$\xi = -1: \qquad N_1(-1) = 1, \qquad N_2(-1) = 0, \qquad N_3(-1) = 0. \tag{7.54}$$

Thus, the following shape functions can be obtained for the second-order line element:

$$N_1(\xi) = -\tfrac{1}{2}\xi(1 - \xi), \tag{7.55}$$

$$N_2(\xi) = (1 + \xi)(1 - \xi), \tag{7.56}$$

$$N_3(\xi) = \tfrac{1}{2}\xi(1 + \xi). \tag{7.57}$$

Next, we calculate the matrix elements shown in Eqs. (7.29)–(7.32).

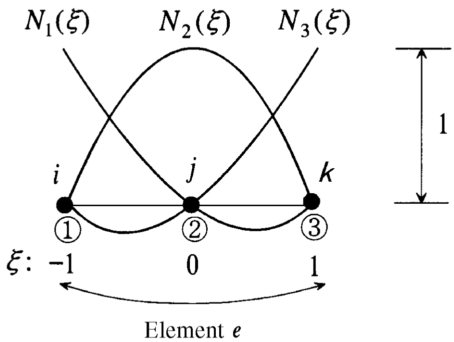

FIGURE 7.4. Second-order line element.

1. $\int_e (d[N_e]/dx)(d[N_e]^T/dx)\, dx$ From Eq. (7.49), we get

$$\frac{d\xi}{dx} = \frac{2}{L_e}$$

and therefore,

$$dx = \tfrac{1}{2} L_e \, d\xi. \tag{7.58}$$

Since the relations

$$\frac{dN_1}{d\xi} = \xi - \tfrac{1}{2}, \tag{7.59}$$

$$\frac{dN_2}{d\xi} = -2\xi, \tag{7.60}$$

$$\frac{dN_3}{d\xi} = \xi + \tfrac{1}{2} \tag{7.61}$$

hold, we get

$$\frac{d[N_e]}{dx} = \frac{d\xi}{dx}\frac{d[N_e]}{d\xi} = \frac{2}{x_k - x_i}\begin{bmatrix} \xi - \frac{1}{2} \\ -2\xi \\ \xi + \frac{1}{2} \end{bmatrix} = \frac{1}{x_k - x_i}\begin{bmatrix} 2\xi - 1 \\ -4\xi \\ 2\xi + 1 \end{bmatrix}. \tag{7.62}$$

Thus, we get

$$\int_e \frac{d[N_e]}{dx}\frac{d[N_e]^T}{dx}\,dx$$

$$= \frac{1}{(x_k - x_i)^2}\int_{-1}^{1}\begin{bmatrix} 2\xi - 1 \\ -4\xi \\ 2\xi + 1 \end{bmatrix}[2\xi - 1 \quad -4\xi \quad 2\xi + 1]\frac{(x_k - x_i)}{2}\,d\xi$$

$$= \frac{1}{2(x_k - x_i)}$$

$$\times \int_{-1}^{1}\begin{bmatrix} (2\xi - 1)^2 & (2\xi - 1)(-4\xi) & (2\xi - 1)(2\xi + 1) \\ -4\xi(2\xi - 1) & (-4\xi)^2 & (-4\xi)(2\xi + 1) \\ (2\xi - 1)(2\xi + 1) & (2\xi + 1)(-4\xi) & (2\xi + 1)^2 \end{bmatrix} d\xi$$

$$= \frac{1}{2(x_k - x_i)}\frac{1}{3}\begin{bmatrix} 14 & -16 & 2 \\ -16 & 32 & -16 \\ 2 & -16 & 14 \end{bmatrix}.$$

This equation is summarized as

$$\int_e \frac{d[N_e]}{dx}\frac{d[N_e]^T}{dx}\,dx = \frac{1}{6L_e}\begin{bmatrix} 14 & -16 & 2 \\ -16 & 32 & -16 \\ 2 & -16 & 14 \end{bmatrix}. \tag{7.63}$$

2. $\int_e [N_e][N_e]^T\,dx$ Through a similar procedure, we get

$$\int_e [N_e][N_e]^T\,dx$$

$$= \int_{-1}^{1}\begin{bmatrix} -\frac{1}{2}\xi(1-\xi) \\ (1+\xi)(1-\xi) \\ \frac{1}{2}\xi(1+\xi) \end{bmatrix}[-\tfrac{1}{2}\xi(1-\xi) \;\; (1+\xi)(1-\xi) \;\; \tfrac{1}{2}\xi(1+\xi)]$$

$$\times [\tfrac{1}{2}(x_k - x_i)]\,d\xi$$

$$= \frac{L_e}{2}\int_{-1}^{1}\begin{bmatrix} \frac{1}{4}\xi^2(1-\xi)^2 & -\frac{1}{2}\xi(1+\xi)(1-\xi)^2 & -\frac{1}{4}(1+\xi)(1-\xi) \\ -\frac{1}{2}\xi(1-\xi)^2(1+\xi) & (1+\xi)^2(1-\xi)^2 & \frac{1}{2}\xi(1+\xi)^2(1-\xi) \\ -\frac{1}{4}\xi^2(1+\xi)(1-\xi) & \frac{1}{2}\xi(1+\xi)^2(1-\xi) & \frac{1}{4}\xi^2(1+\xi)^2 \end{bmatrix} d\xi$$

$$= \frac{L_e}{2}\frac{1}{15}\begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix} = \frac{L_e}{30}\begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}. \tag{7.64}$$

Since Eqs. (7.63) and (7.64) can be used to construct the matrixes [*P*], [*Q*], and [*R*], the eigenenergy can be calculated from the eigenvalue matrix equation (7.35).

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