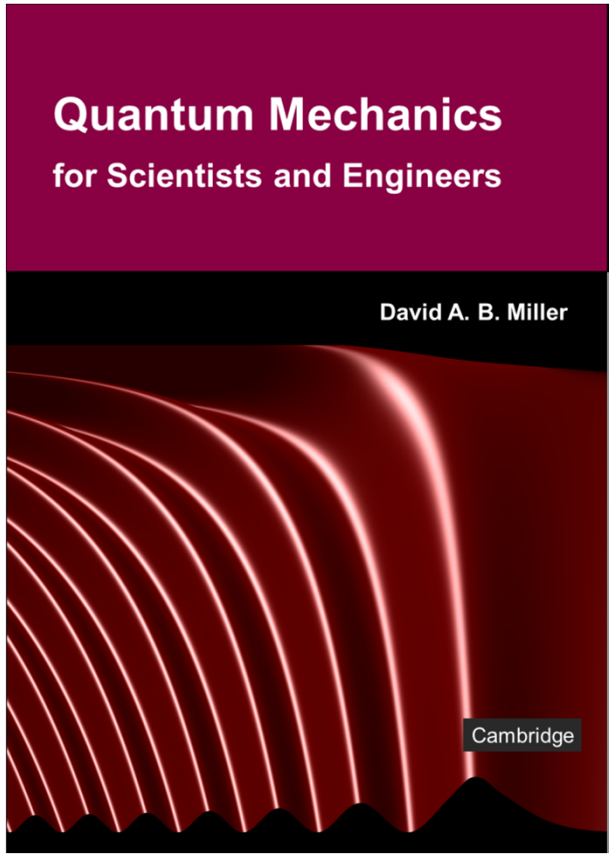
8.2 Approximation methods

Slides: Video 8.2.4 Use of finite matrices

Text reference: Quantum Mechanics for Scientists and Engineers

Section 6.2



Approximation methods

Use of finite matrices

Quantum mechanics for scientists and engineers

David Miller

Finite matrix method for an electron in a well with field

We will need to construct the matrix of the Hamiltonian for this problem

The matrix elements are

$$H_{ij} \equiv \left\langle \psi_i \middle| \hat{H} \middle| \psi_j \right\rangle$$

$$= -\frac{1}{\pi^2}\int_0^1 \psi_i^*(\xi)\frac{d^2}{d\xi^2}\psi_j(\xi)\,d\xi + \mathrm{f}\int_0^1 \psi_i^*(\xi)(\xi - 1/2)\psi_j(\xi)\,d\xi$$

In this particular case

because the wavefunctions are real

the complex conjugation makes no difference

Finite matrix method for an electron in a well with field

In the integral

$$H_{ij} = -\frac{1}{\pi^2}\int_0^1 \psi_i^*(\xi)\frac{d^2}{d\xi^2}\psi_j(\xi)d\xi + \mathrm{f}\int_0^1 \psi_i^*(\xi)(\xi - 1/2)\psi_j(\xi)d\xi$$

if we choose the energy eigenfunctions of the "unperturbed" problem to form our basis set

$$\psi_n(\xi) = \sqrt{2}\sin(n\pi\xi)$$

we can easily perform the derivative analytically

The resulting integrations can be solved analytically also

or they can just be performed numerically

Finite matrix method for an electron in a well with field

For our explicit example here,

we consider a field of 3 dimensionless units, i.e., $\mathsf{f} = 3$

with the first three energy eigenfunctions of the "unperturbed" problem as our finite basis subset

then, evaluating the matrix elements H_{ij}

gives the Hamiltonian matrix

$$\hat{H} = \begin{bmatrix} 1 & -0.54 & 0 \\ -0.54 & 4 & -0.584 \\ 0 & -0.584 & 9 \end{bmatrix}$$

which is Hermitian, as expected

Finite matrix method for an electron in a well with field

Now we numerically find the eigenvalues of this matrix

$$\eta_1 = 0.904,\ \eta_2 = 4.028,\ \eta_3 = 9.068$$

which are close to the "unperturbed" (zero field) values

which would be 1, 4, and 9, respectively

We see also that the lowest energy eigenvalue has reduced from its unperturbed value

These can be compared with the results from the exact ("Airy function") solutions

$$\varepsilon_1 \simeq 0.90419,\ \varepsilon_2 \simeq 4.0275,\ \varepsilon_3 \simeq 9.0173$$

Finite matrix method for an electron in a well with field

The corresponding eigenvectors are solved numerically as

$$|\phi_1\rangle = \begin{bmatrix} 0.985 \\ 0.174 \\ 0.013 \end{bmatrix} \quad |\phi_2\rangle = \begin{bmatrix} -0.175 \\ 0.978 \\ 0.115 \end{bmatrix} \quad |\phi_3\rangle = \begin{bmatrix} 0.007 \\ -0.115 \\ 0.993 \end{bmatrix}$$

Note these are normalized

with the sum of the squares of the elements of the vectors each adding to 1

So, explicitly, the first eigenfunction is

$$\phi_1(\xi) = 0.985\sqrt{2}\sin(\pi\xi) + 0.174\sqrt{2}\sin(2\pi\xi) + 0.013\sqrt{2}\sin(3\pi\xi)$$

Calculated wavefunction

Here is a comparison of

Unperturbed - i.e., no field

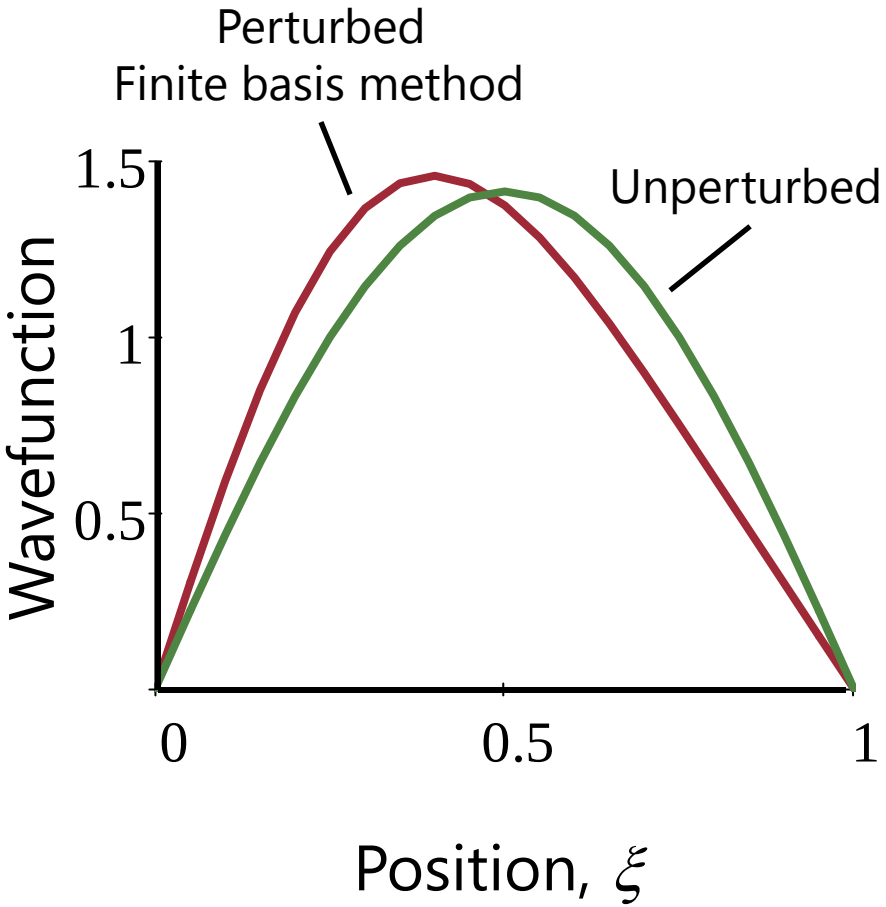
Perturbed - 3 units of field

(finite basis method)

The electron wavefunction has moved to the left with field

Adding more elements to the finite basis

makes negligible change to the calculated eigenvalue



Calculated probability density

For probability density, we compare

Unperturbed - i.e., no field

Perturbed - 3 units of field

(finite basis method)

The electron probablity density has moved to the left with field