FEM formulation for Schrödinger equation

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September 7, 2011

1 Weak form deduction

Consider the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi,$$

being $\hat{H}$ the Hamiltonian Operator $(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}))$. $-\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator and $V(\vec{x})$ is the potential energy.

If we assume

$$\Psi = \Psi e^{-i\omega t}$$

we get

$$i\hbar(-i\omega e^{-i\omega t}\Psi) = \hat{H}e^{-i\omega t}$$

which yields

$$\hbar\omega\Psi = \hat{H}\Psi$$

and is the time-independent Shcrödinger equation, usually written as

$$E\Psi = \hat{H}\Psi \quad (E = \hbar\omega = h\nu) \ . \tag{1}$$

For the FEM solution, let's multiply by a test function v and integrate over the domain Ω

$$\int_\Omega E\Psi v d\Omega = \int_\Omega \hat{H}\Psi v d\Omega$$

or

$$E\int_\Omega \Psi(x)v(x)d\Omega = -\frac{\hbar^2}{2m}\int_\Omega \nabla^2\Psi(x)v(x)d\Omega + \int_\Omega V(x)\Psi(x)v(x)d\Omega \ . \tag{2}$$

(2) could be rewritten, via Green's theorem, as

$$E\int_\Omega \Psi(x)v(x)d\Omega = \frac{\hbar^2}{2m}\int_\Omega \nabla\Psi(x)\nabla v(x)d\Omega + \int_\Omega V(x)\Psi(x)v(x)d\Omega - \int_\Gamma v(x)\frac{\partial\Psi(x)}{d\vec{n}}d\Gamma \quad \text{with } \Gamma = \partial\Omega$$

The term $\int_\Omega v(x)\frac{\partial\Psi(x)}{d\vec{n}}\partial\Omega$ won't make any contribution to the discrete operators (matrices) of the system, so let us consider just

$$E\int_\Omega \Psi(x)v(x)d\Omega = \frac{\hbar^2}{2m}\int_\Omega \nabla\Psi(x)\nabla v(x)d\Omega + \int_\Omega V(x)\Psi(x)v(x)d\Omega \tag{3}$$

2 Approximated functions: interpolation

Functions $\Psi(x)$ and $v(x)$ need to be approximated as

$$\Psi(x) = \sum_{i=1}^{n}\Psi_i N_i(x), \quad \text{with } \Psi_i = \Psi(x_i);$$

$$v(x) = \sum_{i=1}^{n} v_i N_i(x), \quad \text{with } v_i = v(x_i);$$

being these interpolation calculated over the (disjoint) elements.
Since $V(x)$ is the potential, it is known, and two approximations could be applied:

- Assume $V(x)$ constant over each element, or
- Interpolate it with the form functions $N_i(x)$.

Equation (3) could be stated as

$$\frac{\hbar^2}{2m}\sum_{el=1}^{N_{el}}\int_\Omega \nabla\Psi(x)\nabla v(x)d\Omega + \sum_{el=1}^{N_{el}}\int_\Omega V(x)\Psi(x)v(x)d\Omega = E\sum_{el=1}^{N_{el}}\int_\Omega \Psi(x)v(x)d\Omega \ ,$$

where el is a label for the elements.
Therefore, we need to compute it for a single element and then assemble.

$$\frac{\hbar^2}{2m}\sum_{el=1}^{N_{el}}\int_\Omega \nabla\Psi(x)\nabla v(x)d\Omega + \sum_{el=1}^{N_{el}}\int_\Omega V(x)\Psi(x)v(x)d\Omega = E\sum_{el=1}^{N_{el}}\int_\Omega \Psi(x)v(x)d\Omega \ ,$$

So, for each element we have

$$\frac{\hbar}{2m}\int_{\Omega_{el}} \nabla\Psi(x)\nabla v(x)d\Omega_{el} + \int_{\Omega_{el}} V(x)\Psi(x)v(x)d\Omega_{el} = E\int_{\Omega_{el}} \Psi(x)v(x)d\Omega_{el} \ . \tag{4}$$

Then, the approximate functions are replaced in (4). Two approximated versions of equation (4) are given

- assuming the potential $V(x)$ constant over the element, or
- using the same interpolation functions for $V(x)$.

2.1 Potential constant over the element

The resulting equation is

$$\frac{\hbar}{2m}\int\limits_{\Omega_{el}} \Psi_i v_j \nabla N_i(x) \nabla N_j(x) d\Omega_{el} + V(x_m) \int\limits_{\Omega_{el}} \Psi_i v_j N_i(x) N_j(x) d\Omega_{el} = E \int\limits_{\Omega_{el}} \Psi_i v_j N_i(x) N_j(x) d\Omega_{el} \ , \tag{5}$$

where x_m is the centroid of the element.

2.2 Potential interpolated over the element

The resulting equation is

$$\frac{\hbar}{2m}\int\limits_{\Omega_{el}} \Psi_i v_j \nabla N_i(x) \nabla N_j(x) d\Omega_{el} + \int\limits_{\Omega_{el}} V_i \Psi_i v_j N_i^2(x) N_j(x) d\Omega_{el} = E \int\limits_{\Omega_{el}} \Psi_i v_j N_i(x) N_j(x) d\Omega_{el} \ . \tag{6}$$

3 Discrete form

Equation (4) could be written in an abstract (inner-product) fashion like

$$\langle \mathbb{K}\boldsymbol{\Psi}, \mathbf{v} \rangle + \langle \mathbb{V}\boldsymbol{\Psi}, \mathbf{v} \rangle = E \langle \mathbb{M}\boldsymbol{\Psi}, \mathbf{v} \rangle \ ,$$

this is the same that

$$\langle \mathbb{K}\boldsymbol{\Psi} + \mathbb{V}\boldsymbol{\Psi} - E\mathbb{M}\boldsymbol{\Psi}, \mathbf{v} \rangle = 0 \ ,$$

and since $v(x)$ is an *arbitrary* function the vector $\mathbf{v}$ it's too. As a consequence we have

$$\mathbb{K}\boldsymbol{\Psi} + \mathbb{V}\boldsymbol{\Psi} = E\mathbb{M}\boldsymbol{\Psi},$$

The final discrete system, with boundary conditions, will take the form

$$\mathbb{K}\boldsymbol{\Psi} + \mathbb{V}\boldsymbol{\Psi} = E\mathbb{M}\boldsymbol{\Psi} + \mathbf{d} + \mathbf{q}$$

where $\mathbb{K}$ is the equivalent *kinetic energy operator* (stiffness matrix), $\mathbb{V}$ is the *potential energy operator*, $\mathbb{M}$ is the *momentum operator* (mass matrix), $\mathbf{d}$ is the vector with Dirichlet's conditions and $\mathbf{q}$ is the vector with Neumann's conditions.
In quantum mechanics Neumann's boundary conditions don't have a great physical meaning and the most common Dirichlet's conditions are the homogeneous ones, furthermore one is interested in the values of E and the functions Ψ that satisfy the original equation. So the discrete system to solve is

$$\mathbb{K}\boldsymbol{\Psi}_n + \mathbb{V}\boldsymbol{\Psi}_n = E_n\mathbb{M}\boldsymbol{\Psi}_n \ , \tag{7}$$

or

$$\hat{\mathbb{K}}\boldsymbol{\Psi}_n = E_n\mathbb{M}\boldsymbol{\Psi}_n \ ,$$

where E_n is the nth eigenvalue of the system and $\boldsymbol{\Psi}_n$ the nth eigenvector, and $\hat{\mathbb{K}}$ is an equivalent *stiffness* matrix.

4 Matrix computation

The stiffness and mass matrices, for a single element, could be computed as

$$\mathbb{K}_{ij}^{(el)} = \frac{\hbar}{2m} \int_{\Omega_{el}} \nabla N_i \nabla N_j d\Omega_{el}$$

$$\mathbb{M}_{ij}^{(el)} = \int_{\Omega_{el}} N_i N_j d\Omega_{el}$$

4.1 Potential constant over the element

With constant $V(x)$ over each element, the potential matrix is

$$\mathbb{V}_{ij}^{(el)} = V(x_m)\mathbb{M}_{ij}^{(el)}, \quad \text{with } x_m \text{ the centroid of each element } .$$

4.2 Potential interpolated over the element

In this case the potential energy operator is

$$\mathbb{V}_{ij}^{(el)} = \int_{\Omega_{el}} V(x_i) N_i^2 N_j d\Omega_{el}$$

4.3 1D - Linear elements

The functions $N(r)$ are

$$N = \begin{pmatrix} 1-r \\ r \end{pmatrix}$$

so

$$\mathbb{K}_{ij}^{(el)} = \frac{\hbar}{2m} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad \mathbb{M}_{ij}^{(el)} = \frac{1}{6} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \ ,$$

and

$$\mathbb{V}_{\text{constant}}^{(el)} = V(x_m)\mathbb{M}^{(el)} \ .$$

Making $V^{(el)} = (V_1, V_2)$, the value for the potential in each node, we get

$$\mathbb{V}_{\text{interpolated}}^{(el)} = \frac{1}{12} \begin{pmatrix} 3V_1 & V1 \\ V_2 & 3V_2 \end{pmatrix} \ .$$

4.3.1 Global Matrices

(This is not clear in my mind)
The global *equivalent stiffness* matrix is computed as

$$\begin{aligned}
\mathbb{K}_{ii} &= \left(\frac{1}{L_{i-1}} + \frac{1}{L_i}\right)\frac{\hbar}{2m} + \frac{1}{3}[V_{i-1}L_{i-1} + V_i L_i] \qquad \forall\ i \neq 1, i \neq n\ , \\
\mathbb{K}_{ii+1} &= \left[-\frac{1}{L_{i-1}}\frac{\hbar}{2m} + L_{i-1}\frac{V_{i-1}}{6}\right] = \mathbb{K}_{i+1i} \qquad \forall\ i \neq n, \text{ and} \\
\mathbb{K}_{11} &= \left[\frac{1}{L_1}\frac{\hbar}{2m} + L_1\frac{V_1}{3}\right]\ , \\
\mathbb{K}_{nn} &= \left[\frac{1}{L_{n-1}}\frac{\hbar}{2m} + L_{n-1}\frac{V_{n-1}}{3}\right]\ ,
\end{aligned}$$

being L_i the length of the ith element, if the mesh has a constant size so the previous expressions are simpler.
The global mass matrix is computed as

$$\begin{aligned}
\mathbb{M}_{ii} &= \frac{L_i + L_{i+1}}{3} \qquad \forall\ i \neq 1, i \neq n\ , \\
\mathbb{M}_{ii+1} &= \frac{L_i}{6} = \mathbb{M}_{i+1i} \qquad \forall\ i \neq n, \text{ and} \\
\mathbb{M}_{11} &= \frac{L_1}{3}\ , \\
\mathbb{K}_{nn} &= \frac{L_{n-1}}{3}\ ,
\end{aligned}$$

4.4 2D - Linear elements

The functions $N(r, s)$ are

$$N = \begin{pmatrix} 1 - r - s \\ r \\ s \end{pmatrix}$$

so

$$\mathbb{K}^{(el)}_{ij} = \frac{\hbar}{4m}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \quad \mathbb{M}^{(el)}_{ij} = \frac{1}{24}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}\ ,$$

and

$$\mathbb{V}^{(el)}_{\text{constant}} = V(x_m)\mathbb{M}^{(el)}\ .$$

Making $V^{(el)} = (V_1, V_2, V_3)$, the value for the potential in each node, we get

$$\mathbb{V}^{(el)}_{\text{interpolated}} = \frac{1}{60}\begin{pmatrix} 3V_1 & V_1 & V_1 \\ V_2 & 3V_2 & V_2 \\ V_3 & V_3 & 3V_3 \end{pmatrix}\ .$$

4.5 3D - Linear elements

The functions $N(r,s,t)$ are

$$N = \begin{pmatrix} 1-r-s-t \\ r \\ s \\ t \end{pmatrix}$$

so

$$\mathbb{K}_{ij}^{(el)} = \frac{\hbar}{6m}\begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbb{M}_{ij}^{(el)} = \frac{1}{60}\begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 4 & 3/2 & 3 \\ 0 & 3/2 & 2 & 3/2 \\ -1 & 3 & 3/2 & 4 \end{pmatrix},$$

and

$$\mathbb{V}_{\text{constant}}^{(el)} = V(x_m)\mathbb{M}^{(el)} \ .$$

Making $V^{(el)} = (V_1, V_2, V_3, V4)$, the value for the potential in each node, we get

$$\mathbb{V}_{\text{interpolated}}^{(el)} = \frac{1}{360}\begin{pmatrix} 0 & 5V_1 & 2V_1 & 5V_1 \\ -5V_2 & 15V_2 & 4V_2 & 10V_2 \\ 0 & 3V_3 & 6V_3 & 3V_3 \\ -5V_4 & 10V_4 & 4V_4 & 15V_4 \end{pmatrix} \ .$$