

Computational Physics

Project – 2D FEM Schrödinger solver

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1 Background

2 Theory and methods

The two-dimensional time-independent Schrödinger equation is given by

$$-\frac{\hbar}{2m} \left(\frac{\partial^2 \psi(x,y)}{\partial x^2} + \frac{\partial^2 \psi(x,y)}{\partial y^2} \right) + V(x,y)\psi(x,y) = E\psi(x,y). \quad (1)$$

In order to use FEM to numerically solve Eq. (1), we expand the wave function $\psi(x,y)$ in a basis of tetrahedral hat functions $\{\phi_i\}_{i=1..N}$ as

$$\psi(x,y) \approx \sum_{i=1}^N \alpha_i \phi_i(x,y), \quad (2)$$

where N is the number of finite elements used in our computation and α_i , the coefficients in the linear combination are to be solved for. The linear combination then allows us to construct an approximate solution to the original problem. Setting, for simplicity, $\frac{\hbar}{m} = 1$, writing the partial derivatives more concisely as $\nabla^2 \psi(x,y)$, and substituting our basis expansion in Eq. (1), we get

$$\left(-\frac{1}{2} \nabla^2 + V(x,y) \right) \sum_{i=1}^N \alpha_i \phi_i(x,y) = E \sum_{i=1}^N \alpha_i \phi_i(x,y). \quad (3)$$

Rearranging and multiplying both sides by the basis function ϕ_j , we acquire

$$\sum_{i=1}^N \left[-\frac{1}{2} \phi_j(x,y) \nabla^2 \phi_i(x,y) + \phi_j(x,y) V(x,y) \phi_i(x,y) \right] \alpha_i = E \sum_{i=1}^N \alpha_i \phi_j(x,y) \phi_i(x,y). \quad (4)$$

We can now integrate both sides over the domain Ω of our problem (and lighten the notation by getting rid of the cluttering (x, y) -silliness) to get

$$\sum_{i=1}^N \left[-\frac{1}{2} \left(\int_{\Omega} \phi_j \nabla^2 \phi_i \, dA \right) + \left(\int_{\Omega} \phi_j V \phi_i \, dA \right) \right] \alpha_i = \sum_{i=1}^N E \left(\int_{\Omega} \phi_j \phi_i \, dA \right) \alpha_i. \quad (5)$$

The integrals inside the ordinary parentheses are now matrices. The first of the three still needs to be rewritten by Green's first identity:

$$\int_{\Omega} \phi_j \nabla^2 \phi_i \, dA = \underbrace{\oint_{\partial\Omega} \phi_j (\nabla \phi_i \cdot \hat{n}) \, dl}_{=0} - \int_{\Omega} \nabla \phi_j \cdot \nabla \phi_i \, dA, \quad (6)$$

where the vanishing of the indicated term can be achieved in practice by setting either the basis functions $\{\phi_i\}_i$ or the normal-directional derivatives $\{\nabla \phi_i \cdot \hat{n}\}_i$ at the boundary $\partial\Omega$ to 0 by use of Dirichlet or Neumann boundary conditions, respectively. We can then finally identify the matrices in Eq. (5) as the kinetic matrix T_{ji} , the potential matrix V_{ji} and the overlap matrix S_{ji} :

$$\sum_{i=1}^N \left[\underbrace{\frac{1}{2} \left(\int_{\Omega} \nabla \phi_j \cdot \nabla \phi_i \, dA \right)}_{T_{ji}} + \underbrace{\left(\int_{\Omega} \phi_j V \phi_i \, dA \right)}_{V_{ji}} \right] \alpha_i = \sum_{i=1}^N E \underbrace{\left(\int_{\Omega} \phi_j \phi_i \, dA \right)}_{S_{ji}} \alpha_i. \quad (7)$$

Since the summations on both sides of the equation are just the j^{th} elements of a matrix-vector product, the elementwise equality implies equality of the resultant vectors and we get

$$(T + V)\alpha = ES\alpha, \quad (8)$$

which is a generalized eigenvalue problem involving our known matrices. Solving this, we acquire as eigenvectors the coefficient vectors α approximating the true eigenstates as per the linear combination (2) and the corresponding approximate energies E of the eigenstates as eigenvalues.

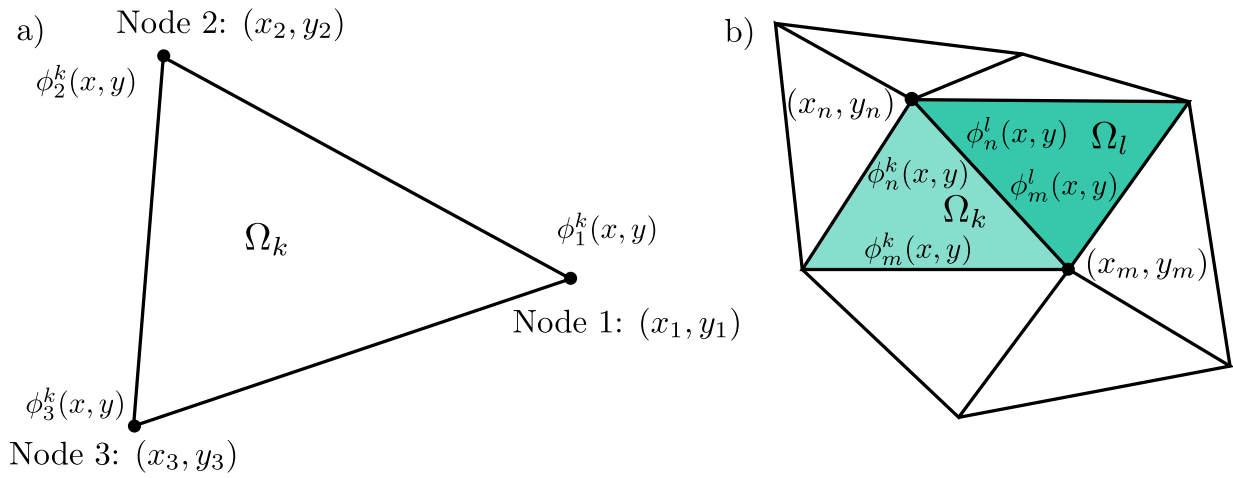


Figure 1: a) A triangular element Ω_k of the domain together with the three vertices or nodes, each being the center of a FEM basis function ϕ . Note that at each triangle, only three basis functions are nonzero, and each of them is affine over Ω_k . b) Illustration of the triangulation. The basis functions centered at (x_n, y_n) and (x_m, y_m) overlap only in two triangular elements Ω_k and Ω_l . Note that in both domains, the functions are affine but not the same as FEM basis functions are piecewise linear.