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

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

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

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

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

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

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

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

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

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

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

$$\int_\Omega \phi_j \nabla^2 \phi_i \,\mathrm{d}A = \underbrace{\oint_{\partial\Omega} \phi_j (\nabla\phi_i \cdot \hat{n}) \,\mathrm{d}l}_{=0} - \int_\Omega \nabla\phi_j \cdot \nabla\phi_i \,\mathrm{d}A, \tag{6}$$

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}:

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

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

$$(T + V)\alpha = ES\alpha, \tag{8}$$

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.