Solving Schrödinger's equation with FEM

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1 Introduction

Quantum mechanics is the modern description of nature, and in particular of the physics at atomic and subatomic scales. Hilbert spaces is the mathematical framework of quantum mechanics, and the physical state or wavefunction is treated as a vector of the space. The state is transformed under operators, which can represent measurable magnitudes such as mass, position or energy, being these called observables. Only the eigenvalues of the observables can be obtained as a measurement. Therefore, the wavefunction 'collapses' to one of the eigenvectors of the observable when the magnitude is measured.

The Hamiltonian operator represents the energy of the system, and it also dictates the dynamics of the state. It is defined as the sum of kinetic and potential energy V and its eigenvectors are the wavefunctions. This constitutes the idea behind the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi\left(x,t\right) + V\left(x\right)\psi\left(x,t\right) = i\hbar\frac{\partial}{\partial t}\psi\left(x,t\right)$$

The term containing the laplacian operator is the kinetic energy (observe that it's equivalent to the classical expression $\frac{p^2}{2m}$ if we define the momentum operator as $p = -i\hbar\nabla$). The quantities involved are $\hbar = \frac{h}{2\pi}$, where $h = 6.62607 \times 10^{-34}$ J/s is the Planck constant, the mass of the particle m, and the wavefunction ψ, which is a distribution of probability. It contains all the information of the system and its modulus $|\psi\left(x,t\right)|^2$ gives the probability of finding the particle at position x at time t when measured.. Therefore, several states are possible before measuring, being this known as the superposition principle.

We can particularize the previous equation for the time independent case and we obtain an eigenvalue equation.

$$-\frac{\hbar^2}{2m}\nabla^2\psi\left(x,t\right) + V\left(x\right)\psi\left(x,t\right) = E\psi\left(x,t\right)$$

Here E is the energy of the system. The low energy eigenstates are of special interest since they are the most present in nature.

In order to see the differences between the quantum and classical theory the particular case of the quantum harmonic oscillator will be studied. The potential energy for the two dimensional harmonic oscillator is given by:

$$V(x,y) = \frac{1}{2}m\omega^2 \left(x^2 + y^2\right)$$

the parameter ω is the angular frequency of the oscillator. To simplify the problem, we will normalize the equation by setting all the constant to 1, which yields the partial differential equation:

$$-\frac{1}{2}\nabla^2\psi\left(x,t\right) + \frac{1}{2}\left(x^2 + y^2\right)\psi\left(x,t\right) = E\psi\left(x,t\right)$$

After applying separation of variables we obtain two equations for each of the spatial components, and the final eigenvectors and eigenvalues are given by

$$\psi_{m,n}\left(x,y\right) = \frac{1}{\sqrt{2^{m+n}m!\,n!\,\pi}}e^{-\frac{x^2+y^2}{2}}H_m\left(x\right)H_n\left(y\right) \quad E_{m,n} = m+n+1$$

The functions $H_m\left(x\right)$ are Hermite polynomials. These are orthogonal polynomials and constitute a basis of the Hilbert space. Moreover, all the states of the harmonic potential are bounded states, meaning that there is a discrete spectrum of energies allowed. The quantization of energy a remarkable difference with respect to the classical theory.

2 Solution of the quantum harmonic oscillator with the FEM

The formulation of the wavefunction as a linear combination of vectors resembles the Gallerkin approximation for the variational form of Finite Element Methods. Taking the same approach as the latter one, the time independent Schrödinger equation can be multiplied by one of the basis functions of the vector space as the test function. Then applying integration by parts and expanding the wavefunction ψ as a linear combination of the basis functions the following equation for the coefficients of the linear combination is obtained:

$$\frac{1}{2}\sum_i \alpha_i \int \nabla\Psi_i \nabla\Psi_j d\bar{x} + \frac{1}{2}\sum_i \alpha_i \int \left(x^2 + y^2\right)\Psi_i\Psi_j d\bar{x} = E\sum_i \alpha_i \int \Psi_i\Psi_j d\bar{x}$$

for $j = 1,...,N$ being N the dimension of the finite dimensional test space V_h. The previous equation can be expressed as a matrix-vector equation:

$$\frac{1}{2}\left(\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots \\ A_{2,1} & A_{2,2} & \cdots \\ \vdots & \vdots & \ddots \\ & & & A_{N,N} \end{bmatrix} + \begin{bmatrix} \widetilde{M}_{1,1} & \widetilde{M}_{1,2} & \cdots \\ \widetilde{M}_{2,1} & \widetilde{M}_{2,2} & \cdots \\ \vdots & \vdots & \ddots \\ & & & \widetilde{M}_{N,N} \end{bmatrix}\right)\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix} = E\begin{bmatrix} M_{1,1} & M_{1,2} & \cdots \\ M_{2,1} & M_{2,2} & \cdots \\ \vdots & \vdots & \ddots \\ & & & M_{N,N} \end{bmatrix}\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}$$

where $A_{i,j} = \int \nabla \Psi_i \nabla \Psi_j d\tilde{x}$, $\widetilde{M}_{i,j} = \int \left(x^2 + y^2 \right) \Psi_i \Psi_j d\tilde{x}$ and $M_{i,j} = \int \Psi_i \Psi_j d\tilde{x}$. The previous equation is a generalized eigenvalue problem of the form $Bx = \lambda Cx$ being both matrices Hermitian. As expected, the eigenvalue λ is the energy E. If the Hermite polynomials were used as a basis the mass matrix (the one containing the scalar product of the basis functions) would become the identity due to the orthonormality properties of Hermite polynomials. However, the choice for the FEM will be a triangulation with linear polynomials $\varphi_l(x, y) = a_l + b_l x + c_l y$ over the nodes $z_{i,j}$, which yields the stiffness matrix and mass matrix:

$$
A = \begin{bmatrix}
T & -\mathbb{I} & & & \\
-\mathbb{I} & T & -\mathbb{I} & & \\
& -\mathbb{I} & \ddots & \ddots & \\
& & \ddots & T & -\mathbb{I} \\
& & & -\mathbb{I} & T
\end{bmatrix}
\qquad
M = \frac{1}{12} \begin{bmatrix}
S & P & & & \\
P^T & S & P & & \\
& P^T & \ddots & \ddots & \\
& & \ddots & S & P \\
& & & P^T & S
\end{bmatrix}
$$

with block matrices

$$
T = \begin{bmatrix}
4 & -1 & & & \\
-1 & 4 & -1 & & \\
& -1 & \ddots & \ddots & \\
& & \ddots & 4 & -1 \\
& & & -1 & 4
\end{bmatrix}
\quad
S = \begin{bmatrix}
6 & 1 & & & \\
1 & 6 & 1 & & \\
& 1 & \ddots & \ddots & \\
& & \ddots & 6 & 1 \\
& & & 1 & 6
\end{bmatrix}
\quad
P = \begin{bmatrix}
1 & 1 & & & \\
& 1 & 1 & & \\
& & \ddots & \ddots & \\
& & & 1 & 1 \\
& & & & 1
\end{bmatrix}
$$

The matrix elements containing the potential will be computed by the integral of the potential times the scalar product of the linear piece-wise functions $\varphi_k \varphi_l$ over the overlapping domains.