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Resolution of the One-Dimensional Scattering Problem by a Finite Element Method

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The finite element method is shown to be very instrumental in obtaining scattering and tunneling solutions of the 1-dimensional Schrödinger equation. Computation of the wavefunction amounts to solving two linear banded systems. In the treatment of tunneling problems, this new method is found more efficient than two finite difference schemes presented previously.
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I. INTRODUCTION

Applications of the finite element method (FEM) to the resolution of the Schrödinger equation are rather recent and most of them have been concerned with the computation of bound states [1–4]. To our knowledge, the sole finite element treatment of states lying in the continuum part of the energy spectrum is that performed by Nordholm and Backsay [5, 6]. In their work, the wavefunction extends from $x=0$ to $x=+\infty$, and vanishes at $x=0$.

In the present paper, we solve the 1D Schrödinger problem of the scattering of plane waves by a localized potential, e.g., the tunneling through a potential barrier, and describe a simple scheme to compute the transmission coefficient and the wavefunction phase shift. For this purpose, it is necessary to extend the wavefunction range to $(-\infty, +\infty)$, since the electron comes from $-\infty$ and either is reflected to $-\infty$ or is transmitted to $+\infty$.

The latter problem has already been dealt with using a finite difference scheme [7], further improved by the Numerov method [8]. These methods are shown to be highly valuable to overcome the limitations imposed by the semiclassical approaches most often used in this context. We wish however to point out that the FEM is more efficient with respect to memory allocation and computational efficiency than the discrete schemes proposed in previous works.

The interest for treating 1-dimensional scattering problems is clearly illustrated by their use in the recently discovered resonant tunneling in superlattices [9–11], or in the resolution of 3-dimensional tunneling problems by the Green's function

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method [12], which requires a preliminary knowledge of 1-dimensional tunneling wavefunctions, which should be computed using the most effective technique. An extension of the method presented here to 3-dimensional tunneling problems will be published elsewhere [13].

II. Framework

We attempt to numerically solve the Schrödinger equation ($\hbar = 2m = 1$),

$$-\frac{d^2\Psi}{dx^2} + (V(x) - E)\,\Psi(x) = 0 \tag{1}$$

associated with a localized potential, i.e., $V(x) = 0$ for $x < C$ and $x > D$. If the potential is not localized (e.g., for a barrier of gaussian shape), it must be truncated to an interval (C, D) outside which the potential differs negligeably from a constant value. This truncation introduces an error in the results.

Hence, the numerical computation may be restricted to the interval (C, D), as the wavefunction in the zero potential regions is known to be a linear combination of the plane waves

$$e^{+ikx} \quad \text{and} \quad e^{-ikx},$$

where

$$k = \sqrt{E}. \tag{2}$$

The wavefunctions and their derivatives must be continuous at both $x = C$ and $x = D$. For sake of simplicity, we restrict our attention to potentials $V(x)$ which assume identical values (here the zero of energy) at $x < C$ and $x > D$. The technique presented hereafter can easily be generalized to more general situations.

Since we aim at computing the wavefunction of a particle approaching the barrier from $-\infty$, we impose that the wavefunction for $x > D$ is the transmitted wave:

$$\Psi = e^{ik(x-D)}, \qquad x \geqslant D. \tag{3}$$

Solving Eq. (1) in (C, D) and applying the matching conditions yield the coefficients A and B of the incident and reflected waves:

$$\Psi = Ae^{ik(x-C)} + Be^{-ik(x-C)}, \qquad x \leqslant C. \tag{4}$$

III. METHOD

The interval (C, D) is subdivided into N elements (x_i, x_{i+1}), $i=0$ to $N-1$, with $x_0 = C$ and $x_N = D$. Although this is not necessary, we work with elements of equal lengths,

$$x_i = C + ih, \qquad i = 0 \text{ to } N \tag{5}$$

where

$$h = \frac{D-C}{N}.$$

(This uniform mesh has been found sufficiently efficient for our purpose.)

In each element (x_i, x_{i+1}), the wavefunction Ψ is approximated by a cubic polynomial of x, the four coefficients of which being related to the values of Ψ and to its first derivative at the end points of this interval. It is equivalent to express Ψ in a basis of real shape functions Φ_i^0 and Φ_i^1 localized in the intervals $)x_{i-1}, x_{i+1}($ (see Fig. 1):

$$\Psi(x) = \sum_{j=0}^{N} \left[\Psi(x_j)\, \Phi_j^0(x) + \frac{d\Psi(x_j)}{dx}\, \Phi_j^1(x) \right] \tag{6}$$

$$\Phi_j^0(x) = (1-t)^2 (1+2t)$$

$$\Phi_j^1(x) = \text{sign}(x)(1-t^2)t$$

where

$$t = \frac{|x|}{h} \qquad \text{and} \qquad \text{sign}(x) = -1 \quad \text{if} \quad x < 0$$

$$= +1 \quad \text{if} \quad x > 0.$$

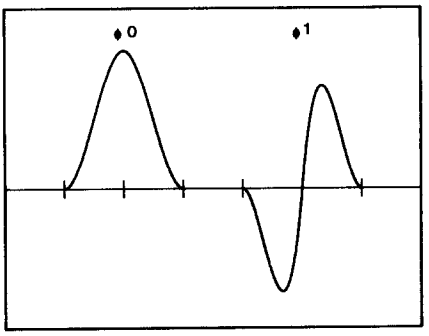

FIG. 1. Shape functions used in the finite-element method. The basis is composed of the two types of shape functions at every point of the discretization mesh.

The Φ_j^0 shape function is somewhat similar to a B-spline [14]: the difference between these two functions is that a B-spline extends over four elements while Φ_j^0 extends over only two elements. The Φ_j^1 shape function, associated with the derivative of Ψ, is typical of the FEM. The reason for choosing these shape functions (rather than, e.g., linear or quadratic shape functions) is that they enable us to match Ψ and its first derivative on the element boundaries.

Galerkin's method [15] yields the so-called weak form of Eq. (1), i.e., only the projection of this equation on all basis functions is required to hold: for $i=0$ to N,

$$\sum_{j=0}^{N}\left[\Psi(x_j)\left\langle \Phi_i^0\left|-\frac{d^2}{dx^2}+V(x)-E\right|\Phi_j^0\right\rangle + \frac{d\Psi(x_j)}{dx}\left\langle \Phi_i^0\left|-\frac{d^2}{dx^2}+V(x)-E\right|\Phi_j^1\right\rangle\right]=0 \tag{7a}$$

$$\sum_{j=0}^{N}\left[\Psi(x_j)\left\langle \Phi_i^1\left|-\frac{d^2}{dx^2}+V(x)-E\right|\Phi_j^0\right\rangle + \frac{d\Psi(x_j)}{dx}\left\langle \Phi_i^1\left|-\frac{d^2}{dx^2}+V(x)-E\right|\Phi_j^1\right\rangle\right]=0 \tag{7b}$$

Equations (7a) and (7b) lead to a system of $2N+2$ linear homogeneous equations with $2N+2$ unknowns.

Due to the fact that all matrix elements of Eqs. (7) are real (the shape functions are real), it is possible to separately compute the real and imaginary parts of Ψ.

A. *Real Part*

From Eq. (3), we know that $\mathrm{Re}(\Psi)$ satisfies a Neumann boundary condition at $x=D$:

$$\frac{d}{dx}[\mathrm{Re}\ \Psi(x_N)]=0. \tag{8}$$

We arbitrarily set

$$\mathrm{Re}\ \Psi(x_0)=1. \tag{9}$$

Consequently, in the system (7), the terms containing $\mathrm{Re}\ \Psi(x_0)$ are transferred to the right-hand sides of the equations, whereas

$$\frac{d}{dx}[\mathrm{Re}\ \Psi(x_N)]$$

vanishes. To determine the $2N$ remaining coefficients of the expansion (6), we only need $2N$ equations: we discard those of Eqs. (7b) involving the bra vectors $\langle\Phi_0^1|$ and $\langle\Phi_N^1|$. So, we obtain a $2N\times 2N$ linear system. The part of $\mathrm{Re}\ (\Psi)$ remaining

in the left-hand side of this system satisfies a Dirichlet boundary condition at $x = C$ and a Neumann boundary condition at $x = D$. (This artificial introduction of boundary conditions generalizes the approach in [6].) These boundary conditions are necessary in order to ensure that the solution of the corresponding differential equation be unique and hence to prevent the linear system becoming singular. The resolution yields

$$\text{Re } \Psi(x_i) \quad \text{and} \quad \text{Re}\left[\frac{d\Psi(x_i)}{dx}\right] \quad \text{for} \quad i = 0 \text{ to } N.$$

Finally, the solution so obtained is renormalized to satisfy

$$\text{Re } \Psi(x_N) = 1 \tag{10}$$

which results from Eq. (3).

B. *Imaginary Part*

The imaginary part is obtained in a very similar way. The only difference is that the unknown part of Im Ψ satisfies a Neumann boundary condition at $x = C$ and a Dirichlet boundary condition at $x = D$. The normalization of Im Ψ results again from Eq. (3):

$$\text{Im}\left[\frac{d\Psi(x_N)}{dx}\right] = k. \tag{11}$$

C. *Transmission Coefficient and Phase Shift*

Since we can determine both the real and imaginary parts of Ψ and its first derivative for $C \leqslant x \leqslant D$, the coefficients A and B of Eq. (4) are immediately derived from the matching conditions at $x = C$. The transmission coefficient T and the phase shift φ are extracted from A [7]:

$$\sqrt{T}\, e^{i\varphi} = \frac{1}{A}. \tag{12}$$

IV. Computational Aspects

Since the basis functions $\Phi_i^0(x)$ and $\Phi_i^1(x)$ are localized in $)x_{i-1}, x_{i+1}($, the matrix element

$$\left\langle \Phi_i^{0/1} \left| -\frac{d^2}{dx^2} + V(x) - E \right| \Phi_j^{0/1} \right\rangle \tag{13}$$

is non-zero only when $|i - j| \leqslant 1$. Hence, the matrices of the $2N \times 2N$ linear systems are banded with a bandwidth equal to 7.

As usual in the FEM, the kinetic part of the matrix element (13) is determined via an integration by parts [16]:

$$\left\langle \Phi_i \left| -\frac{d^2}{dx^2} \right| \Phi_j \right\rangle = \int \frac{d\Phi_i}{dx} \frac{d\Phi_j}{dx} dx. \tag{14}$$

The integrals in Eq. (14) are evaluated analytically accounting for the simple form of the chosen basis functions.

The potential part of the matrix element (13) cannot, in general, be evaluated in closed form. We made use of a three-point Gauss–Legendre quadrature rule to evaluate it on each finite element. In the sample problem considered in Section V, the accuracy on T and φ could not be improved with a five-point quadrature technique. A consequence of this choice of the integration technique is that the potential must be evaluated on a mesh of rather irregularly distributed points. The information concerning the potential is then not quite equivalent to that provided in the finite difference analysis with similar discretization resolution.

V. Results and Comparison with Numerov's Algorithm

We have used the above approach to determine the transmission coefficient T and the phase shift φ of an electron with $E=2$, 7, and 12 tunneling through a model metal–vacuum–metal junction. The potential, including image contributions, is (see Fig. 2)

$$\begin{aligned} V(x) &= 14 - \frac{1}{x+a} - \frac{1}{5-x+a}, \qquad 0 \leqslant x \leqslant 5 \\ V(x) &= 0, \qquad\qquad\qquad\qquad \text{elsewhere.} \end{aligned} \tag{15}$$

a is chosen such that $V(x)=0$ if $x=0$ or $x=5$.

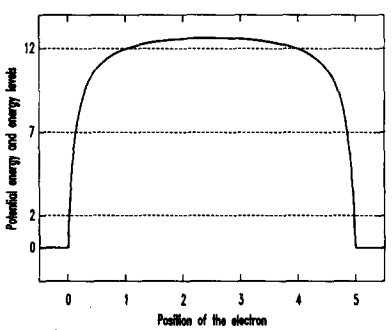

FIG. 2. Potential barrier of the tunneling problem considered in this paper. The horizontal dotted lines are the energy levels for which the transmission coefficient and the phase shift have been computed.

A simple FORTRAN routine implementing this solution is available on request. (Use the electronic mail: LALOYAUX at BNANDP11.)

The same problem has been solved using the finite-difference algorithms developed by Lambin and Vigneron [7, 8]. A comparison between the outcome of the three methods is shown in Tables I and II. The number of steps in each method is chosen to achieve relative errors of 10%, 1%, 0.1%, and 0.01% on T and absolute errors of 0.1, 0.01, and 0.001 radians on φ. The computation times (CPU times) are compared. It occurs that for low accuracies the finite difference schemes may be quicker than the finite elements, even though they require a higher number of steps. Nevertheless, if a higher number of significant digits is required, the FEM becomes the most effective technique, owing to the better convergence of the results as the number of discretization steps is increased. The lower the energy of the tunneling particle, the earlier the crossing over of the finite difference and FEM calculation times occurs.

TABLE I

Comparison between the Number of Steps and the Calculation Time (in CPU Seconds) Needed to Achieve Relative Errors of 10%, 1%, 0.1%, and 0.01% on T with the Finite Element, Continued Fractions and Numerov Methods

Finite element method			*Numerov algorithm*			*Continued fractions*		
N	Time	Transm. coeff.	N	Time	Transm. coeff.	N	Time	Transm. coeff.
$E=2$: Exact $T=0.208112\times10^{-12}$								
		(10^{-12})			(10^{-12})			(10^{-12})
9	0.03	0.227679	10	0.00	0.196217	79	0.02	0.228621
11	0.04	0.208507	343	0.10	0.206091	259	0.06	0.209958
24	0.09	0.207939	1175	0.34	0.207914	804	0.18	0.208303
42	0.15	0.208091	4046	1.15	0.208094	2514	0.58	0.208131
$E=7$: Exact $T=0.271077\times10^{-8}$								
		(10^{-8})			(10^{-8})			(10^{-8})
6	0.02	0.286081	24	0.01	0.245136	46	0.01	0.297792
12	0.04	0.273445	215	0.06	0.268724	149	0.03	0.273554
28	0.10	0.271320	731	0.21	0.270831	455	0.11	0.271342
60	0.22	0.271100	2286	0.65	0.271050	1563	0.36	0.271100
$E=12$: Exact $T=0.489308\times10^{-2}$								
		(10^{-2})			(10^{-2})			(10^{-2})
5	0.02	0.529623	17	0.01	0.441144	36	0.01	0.446634
10	0.04	0.493982	215	0.06	0.493598	113	0.03	0.484659
19	0.07	0.489754	731	0.21	0.489758	377	0.09	0.488887
33	0.12	0.489354	2514	0.71	0.489349	1175	0.28	0.489265

Note. The "exact" values of T are obtained by the FEM with 1000 steps.

TABLE II

Comparison between the Number of Steps and the Calculation Time (in CPU Seconds) Needed to Achieve Absolute Errors of 0.1, 0.01, and 0.001 Radians on φ with the Finite Element, Continued Fractions, and Numerov Methods

Finite element method			*Numerov algorithm*			*Continued fractions*		
N	Time	Phase shift	N	Time	Phase shift	N	Time	Phase shift
$E=2$: Exact $\varphi=-0.407423$								
4	0.02	−0.47721	55	0.02	−0.49940	86	0.02	−0.31206
12	0.04	−0.41574	196	0.06	−0.41607	731	0.18	−0.39757
26	0.10	−0.40825	665	0.19	−0.40836	7165	1.65	−0.40643
$E=7$: Exact $\varphi=0.853125$								
5	0.02	0.76561	14	0.01	0.95046	149	0.03	0.94874
12	0.04	0.84456	236	0.07	0.84338	1421	0.33	0.86251
24	0.09	0.85225	884	0.25	0.85228	13,957	3.32	0.85407
$E=12$: Exact $\varphi=2.63280$								
4	0.02	2.6314	17	0.01	2.5374	179	0.04	2.7326
4	0.02	2.6314	28	0.01	2.6269	1890	0.44	2.6420
16	0.06	2.6338	665	0.19	2.6319	18,575	4.31	2.6337

Note. The "exact" values of φ are obtained by the FEM with 1000 steps.

In the three methods, memory storage and computation time are proportional to the number of discretization elements. This is readily understandable for the finite difference techniques which lead to three-term recurrence equations. The same holds true with the FEM: the bandwidth of the linear system involved is also independent of the discretization size.

The above example shows that the FEM approach is more advisable from the computational point of view than the finite difference schemes advocated earlier to improve upon the usual semi-classical schemes.

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